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* * * * * Welcome to STN International * * * * *

NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	AUG 06	CAS REGISTRY enhanced with new experimental property tags
NEWS	3	AUG 06	FSTA enhanced with new thesaurus edition
NEWS	4	AUG 13	CA/CAPplus enhanced with additional kind codes for granted patents
NEWS	5	AUG 20	CA/CAPplus enhanced with CAS indexing in pre-1907 records
NEWS	6	AUG 27	Full-text patent databases enhanced with predefined patent family display formats from INPADOCDB
NEWS	7	AUG 27	USPATOLD now available on STN
NEWS	8	AUG 28	CAS REGISTRY enhanced with additional experimental spectral property data
NEWS	9	SEP 07	STN AnaVist, Version 2.0, now available with Derwent World Patents Index
NEWS	10	SEP 13	FORIS renamed to SOFIS
NEWS	11	SEP 13	INPADOCDB enhanced with monthly SDI frequency
NEWS	12	SEP 17	CA/CAPplus enhanced with printed CA page images from 1967-1998
NEWS	13	SEP 17	CAPplus coverage extended to include traditional medicine patents
NEWS	14	SEP 24	EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS	15	OCT 02	CA/CAPplus enhanced with pre-1907 records from Chemisches Zentralblatt
NEWS	16	OCT 19	BEILSTEIN updated with new compounds
NEWS	17	NOV 15	Derwent Indian patent publication number format enhanced
NEWS	18	NOV 19	WPIX enhanced with XML display format
NEWS	19	NOV 30	ICSD reloaded with enhancements
NEWS	20	DEC 04	LINPADOCDB now available on STN
NEWS	21	DEC 14	BEILSTEIN pricing structure to change
NEWS	22	DEC 17	USPATOLD added to additional database clusters
NEWS	23	DEC 17	IMSDRUGCONF removed from database clusters and STN
NEWS	24	DEC 17	DGENE now includes more than 10 million sequences
NEWS	25	DEC 17	TOXCENTER enhanced with 2008 MeSH vocabulary in MEDLINE segment
NEWS	26	DEC 17	MEDLINE and LMEDLINE updated with 2008 MeSH vocabulary
NEWS	27	DEC 17	CA/CAPplus enhanced with new custom IPC display formats
NEWS	28	DEC 17	STN Viewer enhanced with full-text patent content from USPATOLD
NEWS	29	JAN 02	STN pricing information for 2008 now available
NEWS	30	JAN 16	CAS patent coverage enhanced to include exemplified prophetic substances
NEWS	31	JAN 28	USPATFULL, USPAT2, and USPATOLD enhanced with new custom IPC display formats
NEWS	32	JAN 28	MARPAT searching enhanced

NEWS 33 JAN 28 USGENE now provides USPTO sequence data within 3 days
of publication
NEWS 34 JAN 28 TOXCENTER enhanced with reloaded MEDLINE segment
NEWS 35 JAN 28 MEDLINE and LMEDLINE reloaded with enhancements

NEWS EXPRESS 19 SEPTEMBER 2007: CURRENT WINDOWS VERSION IS V8.2,
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007.

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items
NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that
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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 09:38:21 ON 07 FEB 2008

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 09:38:26 ON 07 FEB 2008

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STRUCTURE FILE UPDATES: 6 FEB 2008 HIGHEST RN 1001892-66-5

DICTIONARY FILE UPDATES: 6 FEB 2008 HIGHEST RN 1001892-66-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

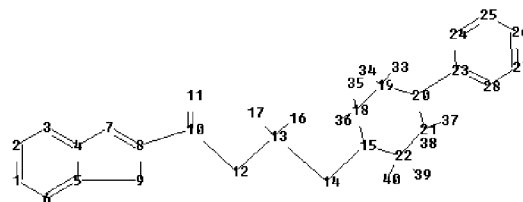
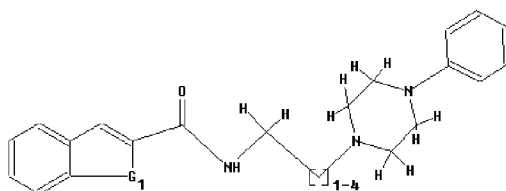
Please note that search-term pricing does apply when
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REGISTRY includes numerically searchable data for experimental and
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experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10519487b.str



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chain nodes :
10 11 12 13 14 16 17 33 34 35 36 37 38 39 40
ring nodes :
1 2 3 4 5 6 7 8 9 15 18 19 20 21 22 23 24 25 26 27 28
chain bonds :
8-10 10-11 10-12 12-13 13-14 13-16 13-17 14-15 18-35 18-36 19-33 19-34
20-23 21-37 21-38 22-39 22-40
ring bonds :
1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-9 7-8 8-9 15-18 15-22 18-19 19-20 20-21
21-22 23-24 23-28 24-25 25-26 26-27 27-28
exact/norm bonds :
4-7 5-9 7-8 8-9 8-10 10-11 10-12 12-13 13-14 13-16 13-17 14-15 15-18
15-22 18-19 18-35 18-36 19-20 19-33 19-34 20-21 20-23 21-22 21-37 21-38
22-39 22-40

normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 23-24 23-28 24-25 25-26 26-27 27-28
isolated ring systems :
containing 1 : 15 : 23 :
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G1:O,S

Match level :

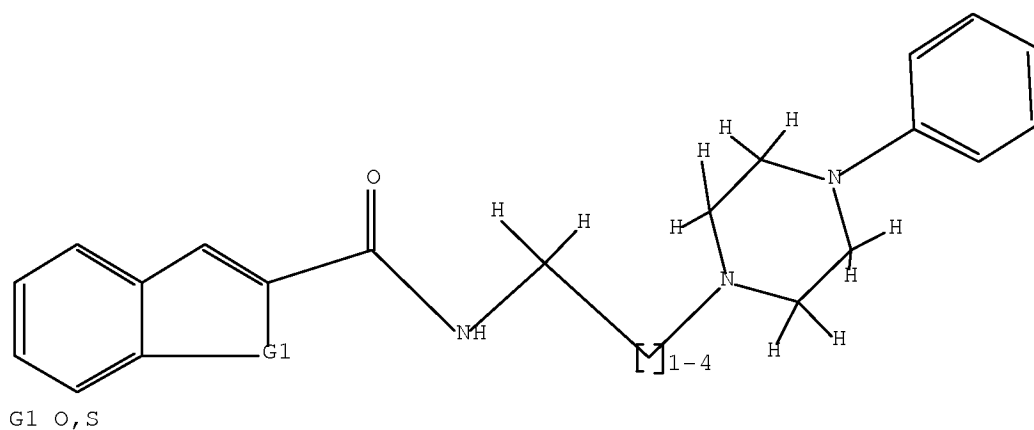
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1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:Atom 16:CLASS 17:CLASS 18:Atom
19:Atom 20:Atom 21:Atom
22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 33:CLASS 34:CLASS
35:CLASS
36:CLASS 37:CLASS 38:CLASS 39:CLASS 40:CLASS
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L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 09:39:49 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 24 TO ITERATE

100.0% PROCESSED 24 ITERATIONS

4 ANSWERS

SEARCH TIME: 00.00.02

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 187 TO 773

PROJECTED ANSWERS: 4 TO 200

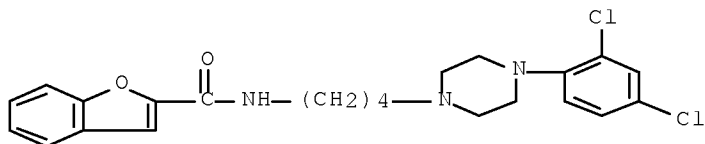
L2 4 SEA SSS SAM L1

=> d scan

L2 4 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN 2-Benzofurancarboxamide, N-[4-[4-(2,4-dichlorophenyl)-1-piperazinyl]butyl]-

MF C23 H25 Cl2 N3 O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> s l1 full

FULL SEARCH INITIATED 09:40:02 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 397 TO ITERATE

100.0% PROCESSED 397 ITERATIONS

91 ANSWERS

SEARCH TIME: 00.00.01

L3 91 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

179.28

179.49

FILE 'CAPLUS' ENTERED AT 09:40:06 ON 07 FEB 2008

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FILE COVERS 1907 - 7 Feb 2008 VOL 148 ISS 6

FILE LAST UPDATED: 6 Feb 2008 (20080206/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> s l3 full

L4 31 L3

=> d ibib abs hitstr tot

L4 ANSWER 1 OF 31 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:817760 CAPLUS Full-text

DOCUMENT NUMBER: 147:211915

TITLE: N-(α -Carbonylamino)acetyl)piperazines as antibacterial agents, their preparation, pharmaceutical compositions, and use in therapy

INVENTOR(S): Hidalgo Rodriguez, Jose; Catena Ruiz, Juan Lorenzo; Masip Masip, Isabel; Serra Comas, Maria del Carmen; Rey Puiggros, Oscar; Lagunas Arnal, Carmen; Salcedo Roca, Carolina; Balsa Lopez, Dolors

PATENT ASSIGNEE(S): Laboratorios Salvat, S.A., Spain

SOURCE: PCT Int. Appl., 54pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007082910	A1	20070726	WO 2007-EP50489	20070118
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
PRIORITY APPLN. INFO.:			ES 2006-158	A 20060119
OTHER SOURCE(S):			MARPAT 147:211915	
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention relates to N-(α -(carbonylamino)acetyl)piperazines of general formula I, which are antibacterial agents. In compds. I, X is O, NH, S, -NHC(O)-, or -NHC(=S)-; R1 and R4 are independently H, (un)substituted C1-4 alkyl, (un)substituted C2-4 alkenyl, or (un)substituted C2-4 alkynyl; R2 is selected from H, OH, NH2, (un)substituted C1-4 alkyl, (un)substituted C1-4 alkoxy, (un)substituted C1-4 alkylamino, (un)substituted 3- to 7-membered monocyclic or 6- to 10-membered bicyclic ring system containing 1 to 3 heteroatoms independently selected from O, S, and N, etc.; R3 is H, (un)substituted C1-4 alkyl, (un)substituted C2-4 alkenyl, (un)substituted C2-4 alkynyl, or 3- to 7-membered monocyclic ring containing 1 to 3 heteroatoms independently selected from O, S, and N, or R3 and R4 may together form (un)substituted 3- to 7-membered monocyclic ring containing 1 to 3 heteroatoms independently selected from O, S, and N; R5 and R6 are independently selected from H and halo; and R7 is H, (un)substituted C1-4 alkyl, (un)substituted C2-4 alkenyl, (un)substituted C2-4 alkynyl, or (un)substituted heteroaryl; including stereoisomers, polymorphs, N-oxides, solvates and salts thereof. The invention also relates to the preparation of I, pharmaceutical compns. comprising a therapeutically effective amount of a compound I and appropriate amts. of one or more pharmaceutically acceptable excipients, as well as to the use of the compns. against bacterial infections in animals, including humans. Amidation of piperazine II (preparation referenced) with N-Boc-glycine followed by deprotection and coupling with 4-nitropyridine-3-carboxylic acid N-oxide to give acylpiperazine III. The compds. of the invention express antibacterial activity, e.g., compound III expressed MIC values of 0.125-0.5 μ g/mL and 0.25-0.5 μ g/mL towards *Streptococcus faecalis* (BCM-010) and *Staphylococcus aureus* (BCM-012), resp.

IT 944723-06-2F, N-[2-[4-[2-Fluoro-4-[5-((isoxazol-3-ylamino)methyl)isoxazol-3-yl]phenyl]piperazin-1-yl]-2-oxoethyl]-benzofuran-2-carboxamide 944724-32-7F, N-[2-[4-[2-Fluoro-4-[5-((isoxazol-3-ylamino)methyl)isoxazol-3-yl]phenyl]piperazin-1-yl]-2-oxoethyl]-5-nitrobenzofuran-2-carboxamide 944724-35-0P, N-[2-[4-[2-Fluoro-4-[5-(hydroxymethyl)isoxazol-3-yl]phenyl]piperazin-1-yl]-2-oxoethyl]-

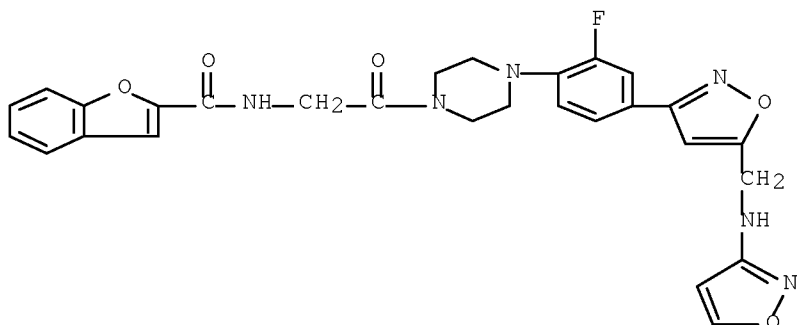
benzofuran-2-carboxamide

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of N-((carbonylamino)acetyl)piperazines as antibacterial agents)

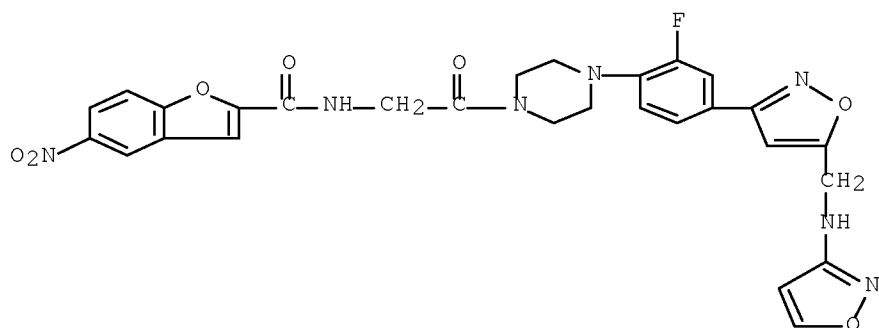
RN 944723-06-2 CAPLUS

CN 2-Benzofurancarboxamide, N-[2-[4-[2-fluoro-4-[5-[(3-isoxazolylamino)methyl]-3-isoxazolyl]phenyl]-1-piperazinyl]-2-oxoethyl]- (CA INDEX NAME)



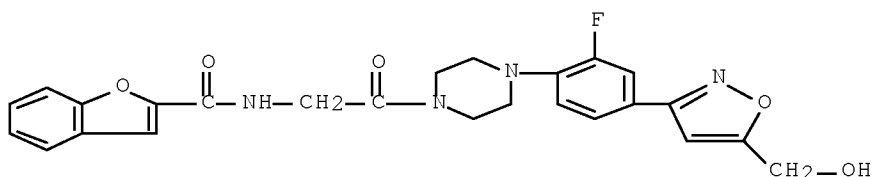
RN 944724-32-7 CAPLUS

CN 2-Benzofurancarboxamide, N-[2-[4-[2-fluoro-4-[5-[(3-isoxazolylamino)methyl]-3-isoxazolyl]phenyl]-1-piperazinyl]-2-oxoethyl]-5-nitro- (CA INDEX NAME)



RN 944724-35-0 CAPLUS

CN 2-Benzofurancarboxamide, N-[2-[4-[2-fluoro-4-[5-(hydroxymethyl)-3-isoxazolyl]phenyl]-1-piperazinyl]-2-oxoethyl]- (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 31 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:18419 CAPLUS Full-text

DOCUMENT NUMBER: 146:308379

TITLE: Structure-Selectivity Investigations of D2-Like Receptor Ligands by CoMFA and CoMSIA Guiding the Discovery of D3 Selective PET Radioligands

AUTHOR(S): Salama, Ismail; Hocke, Carsten; Utz, Wolfgang; Prante, Olaf; Boeckler, Frank; Huebner, Harald; Kuwert, Torsten; Gmeiner, Peter

CORPORATE SOURCE: Department of Medicinal Chemistry, Emil Fischer Center, Friedrich Alexander University, Erlangen, D-91052, Germany

SOURCE: Journal of Medicinal Chemistry (2007), 50(3), 489-500
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 146:308379

AB Elucidation of the physiol. role of the D3 receptor and its distribution in the brain using positron emission tomog. (PET) is hampered by the lack of bioavailable subtype selective tracer ligands. To develop appropriate D3 radioligands, we designed an integrative procedure involving the elucidation of structural features determining D3 selectivity over both congeners D2 and D4 by comparative mol. anal. Thus, we have successfully generated CoMFA and CoMSIA models based on the affinity differences of a series of 79 ligands representing a broad range of selectivities. These models yielded highly significant cross-validations ($q^2_{cv}(D3/D2) = 0.86$; $q^2_{cv}(D3/D4) = 0.92$) and excellent predictions of a 16-ligand test set ($r^2_{pred} = 0.79-0.93$). Exploiting this information, synthesis and receptor binding studies directed us to the fluorinated lead compds. 78 and 79, featuring subnanomolar D3 affinities and considerable selectivities over D2 and D4 and, subsequently, to the subtype selective PET tracers [^{18}F]78 and [^{18}F]79.

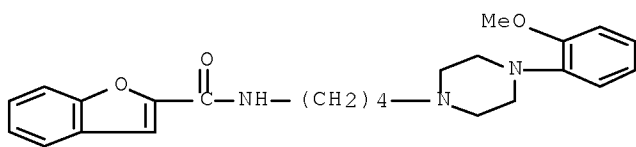
IT 474432-63-8 474432-64-9 474432-65-0
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644988-82-9 644988-83-0 910127-38-7
910127-39-8 910127-41-2 910127-43-4
928658-17-7

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(Structure-Selectivity Investigations of D2-Like Receptor Ligands by CoMFA and CoMSIA Guiding the Discovery of D3 Selective PET Radioligands)

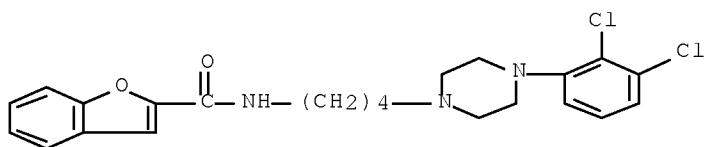
RN 474432-63-8 CAPLUS

CN 2-Benzofurancarboxamide, N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



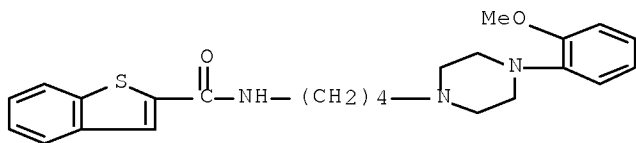
RN 474432-64-9 CAPLUS

CN 2-Benzofurancarboxamide, N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]-
(CA INDEX NAME)



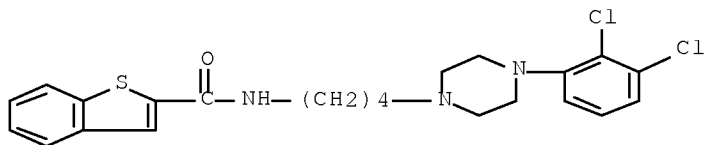
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CN Benzo[b]thiophene-2-carboxamide, N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



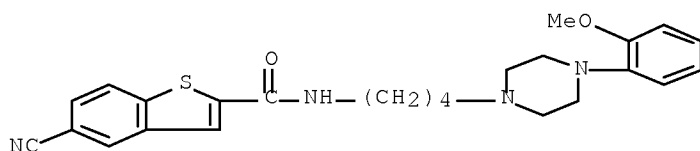
RN 474432-66-1 CAPLUS

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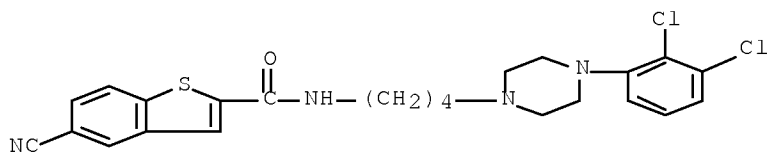
RN 644988-68-1 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, 5-cyano-N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



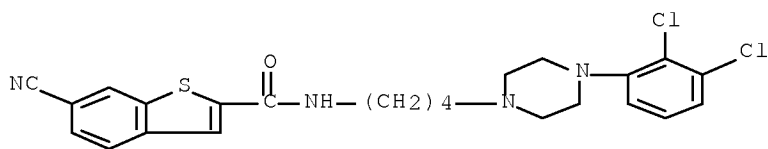
RN 644988-69-2 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, 5-cyano-N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



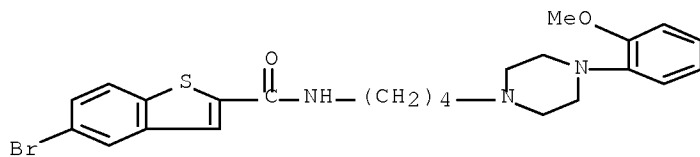
RN 644988-71-6 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, 6-cyano-N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



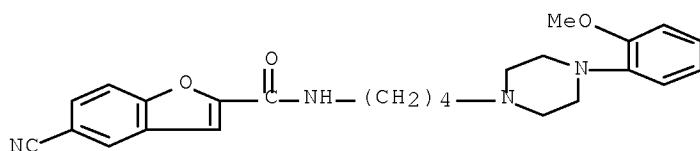
RN 644988-72-7 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, 5-bromo-N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



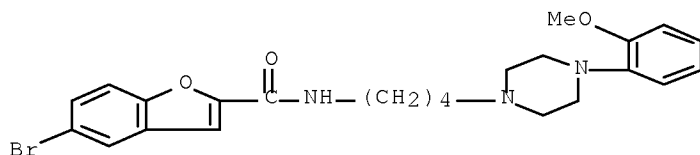
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CN 2-Benzofurancarboxamide, 5-cyano-N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



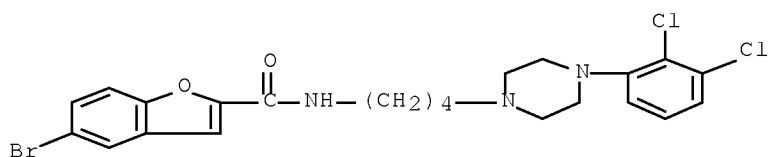
RN 644988-82-9 CAPLUS

CN 2-Benzofurancarboxamide, 5-bromo-N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



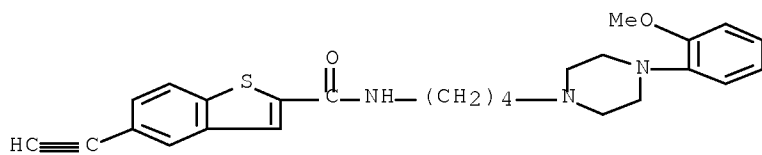
RN 644988-83-0 CAPLUS

CN 2-Benzofurancarboxamide, 5-bromo-N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



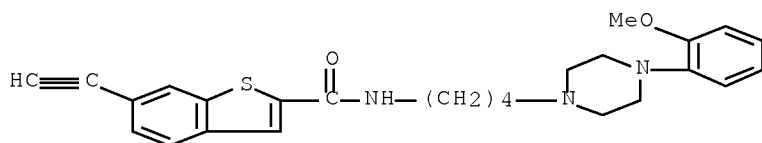
RN 910127-38-7 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, 5-ethynyl-N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



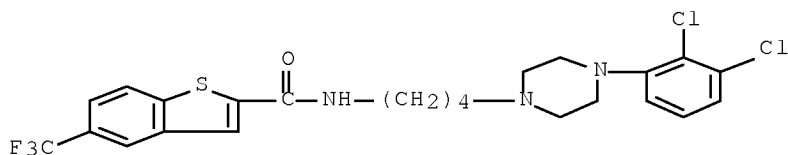
RN 910127-39-8 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, 6-ethynyl-N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



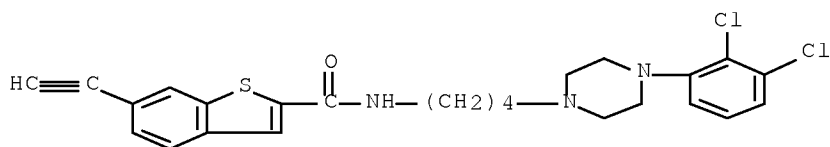
RN 910127-41-2 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]-5-(trifluoromethyl)- (CA INDEX NAME)



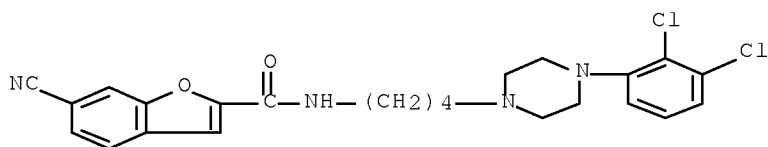
RN 910127-43-4 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]-6-ethynyl- (CA INDEX NAME)



RN 928658-17-7 CAPLUS

CN 2-Benzofurancarboxamide, 6-cyano-N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



REFERENCE COUNT: 72 THERE ARE 72 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 31 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:878985 CAPLUS Full-text

DOCUMENT NUMBER: 146:269023

TITLE: Synthesis and radiolabeling of N-[4-[4-(2-

[11C]methoxyphenyl)piperazin-1-yl]butyl]benzo[b]thiophene-2-carboxamide - a potential radiotracer for D3 receptor imaging with PET

AUTHOR(S): Kuhnast, Bertrand; Valette, Heric; Besret, Laurent; Demphel, Stephane; Coulon, Christine; Ottaviani, Michele; Guillermier, Martine; Bottlaender, Michel; Dolle, Frederic

CORPORATE SOURCE: Service Hospitalier Frederic Joliot, SHFJ/CEA/DSV, Orsay, 91401, Fr.

SOURCE: Nuclear Medicine and Biology (2006), 33(6), 785-795
CODEN: NMBIEO; ISSN: 0969-8051

PUBLISHER: Elsevier Inc.

DOCUMENT TYPE: Journal

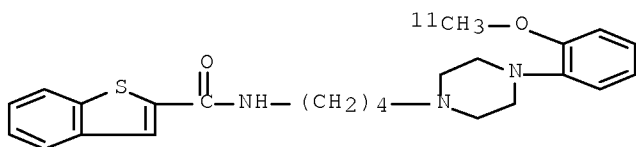
LANGUAGE: English

AB FAUC346 (N-[4-[4-(2-methoxyphenyl)piperazin-1-yl]butyl]benzo[b]thiophene-2-carboxamide), an in vitro D3-selective ligand, and its normethyl derivative have been synthesized from com. available 1-(2-substituted-phenyl)piperazines. FAUC346 has been labeled using [11C]methyl triflate in acetone containing aqueous NaOH (5 Equiv) at -10 °C for 1 min, purified on semipreparative reverse-phase high-performance liquid chromatog. (HPLC) and formulated as an i.v. injectable solution using a Sep-Pak Plus C18 device. Up to 5.5 GBq of [11C]FAUC346 (N-[4-[4-(2-[methyl- 11C]methoxyphenyl)piperazin-1-yl]butyl]benzo[b]thiophene-2-carboxamide), with a specific radioactivity of 45-75 GBq/μmol, could be obtained in 30-35 min, including HPLC purification and formulation starting from 44.4 GBq of [11C]carbon dioxide. Preliminary pharmacol. evaluation of [11C]FAUC346 in rat brain clearly demonstrated in vivo selectivity for D3 receptors and the absence of radiolabeled metabolite within the brain. These encouraging results, however, could not be confirmed in nonhuman primates; therefore, this radioligand does not appear to have the required pharmacol. profile for a positron emission tomog. probe for imaging D3 receptors.

IT 927187-11-9P
RL: DGN (Diagnostic use); PKT (Pharmacokinetics); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(N-[4-[4-(2-[11C]methoxyphenyl)piperazin-1-yl]butyl]benzo[b]thiophene-2-carboxamide preparation as potential tracer for D3 receptor PET imaging)

RN 927187-11-9 CAPLUS

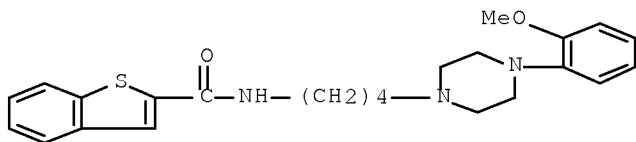
CN Benzo[b]thiophene-2-carboxamide, N-[4-[4-[2-(methoxy-11C)phenyl]-1-piperazinyl]butyl]- (CA INDEX NAME)



IT 474432-65-0P 927187-10-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(N-[4-[4-(2-[11C]methoxyphenyl)piperazin-1-yl]butyl]benzo[b]thiophene-2-carboxamide preparation as potential tracer for D3 receptor PET imaging)

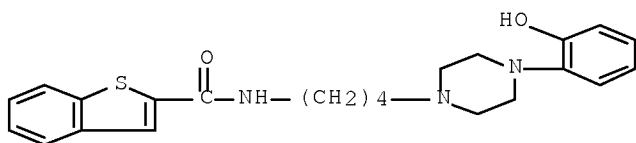
RN 474432-65-0 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



RN 927187-10-8 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, N-[4-[4-(2-hydroxyphenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 31 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:845889 CAPLUS Full-text

DOCUMENT NUMBER: 145:397468

TITLE: Synthesis and biological evaluation of potential positron emission tomography (PET) ligands for brain visualization of dopamine D3 receptors

AUTHOR(S): Lacivita, Enza; Berardi, Francesco; Colabufo, Nicola A.; Leopoldo, Marcello; Perrone, Roberto; Tortorella, Vincenzo

CORPORATE SOURCE: Dipartimento Farmaco-Chimico, Universita degli Studi di Bari, Bari, 70125, Italy

SOURCE: ARKIVOC (Gainesville, FL, United States) (2006), (8), 102-110

CODEN: AGFUAR

URL: http://www.arkat-usa.org/ARKIVOC/JOURNAL_CONTENT/manuscripts/2006/ML-1809GP%20as%20published%20mainmanuscript.pdf

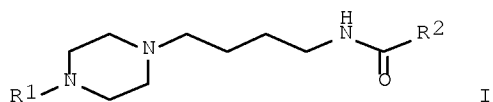
PUBLISHER: Arkat USA Inc.

DOCUMENT TYPE: Journal; (online computer file)

LANGUAGE: English

OTHER SOURCE(S): CASREACT 145:397468

GI



AB The synthesis and binding affinities for dopamine D3 and D2 receptors of several N-[4-(4-aryl piperazin-1-yl)butyl]arylcarboxamides I [R1 = 2-MeOC6H4, 5-methoxybenzisoxazol-3-yl, 2-benzimidazolyl, 7-methoxyisoquinolin-1-yl, etc.; R2 = 7-methoxybenzofuran-2-yl, 4-(4-morpholinyl)phenyl, quinoxalin-6-yl, etc.] are reported. These compds. were designed by the structural modification of the formerly reported D3 receptor ligand I (R1 = 5-methoxybenzisoxazol-3-yl; R2 = 2,3-Cl2C6H3), with the aim to obtain a suitable lipophilicity and the structural features for labeling. Among the studied compds., I [R1 = 5-methoxybenzisoxazol-3-yl; R2 = 4-(4-morpholinyl)phenyl, 4-(1-imidazolyl)phenyl, 5-(2-furyl)pyrazol-3-yl] displayed good D3 receptor affinities (Ki values 38, 22.6, and 21.3 nM, resp.) and were found to be inactive at D2 receptor. Moreover, on the basis of their exptl. log P values and their ability to cross the Caco-2 monolayer, these three compds. are likely to permeate the blood-brain barrier, in contrast to I (R1 = 5-methoxybenzisoxazol-3-yl; R2 = 2,3-Cl2C6H3).

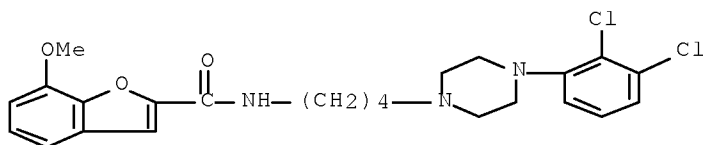
IT 687634-09-9

RL: PAC (Pharmacological activity); PRP (Properties); BIOL (Biological study)

(preparation, calculated lipophilicity and biol. evaluation of N-(aryl piperazinylbutyl) amides as potential positron emission tomog. ligands for brain visualization of dopamine D3 receptors)

RN 687634-09-9 CAPLUS

CN 2-Benzofurancarboxamide, N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]-7-methoxy- (CA INDEX NAME)



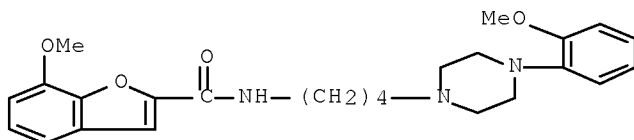
IT 873662-57-8P

RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation, calculated lipophilicity and biol. evaluation of N-(aryl piperazinylbutyl) amides as potential positron emission tomog. ligands for brain visualization of dopamine D3 receptors)

RN 873662-57-8 CAPLUS

CN 2-Benzofurancarboxamide, 7-methoxy-N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



REFERENCE COUNT:

17

THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 31 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:739370 CAPLUS Full-text

DOCUMENT NUMBER: 145:347791

TITLE: CoMFA and CoMSIA investigations of dopamine D3 receptor ligands leading to the prediction, synthesis, and evaluation of rigidized FAUC 365 analogues

AUTHOR(S): Salama, Ismail; Schlotter, Karin; Utz, Wolfgang; Huebner, Harald; Gmeiner, Peter; Boeckler, Frank

CORPORATE SOURCE: Department of Medicinal Chemistry, Emil Fischer Center, Friedrich Alexander University, Erlangen, D-91052, Germany

SOURCE: Bioorganic & Medicinal Chemistry (2006), 14(17), 5898-5912

CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 145:347791

AB Taking advantage of our inhouse exptl. data on dopamine D3 receptor modulators, we have successfully established highly significant CoMFA and CoMSIA models ($q^2_{cv} = 0.82/0.76$). These models were carefully investigated to assure their stability and predictivity ($r^2_{pred} = 0.65/0.61$) and subsequently applied to guide exptl. investigations on the synthesis and receptor binding of three conformationally restricted D3 ligands. Besides the high D3 affinity, the test compound 45, incorporating a trans-1,4-cyclohexylene partial structure, exhibited improved (.apprx.3200-fold) selectivity over the D4 subtype.

IT 474432-63-8 474432-64-9 474432-65-0

474432-66-1 474432-66-1D, FAUC365, analogs

644988-68-1 644988-69-2 644988-70-5

644988-71-6 644988-72-7 644988-73-8

644988-81-8 644988-82-9 644988-83-0

910127-38-7 910127-39-8 910127-40-1

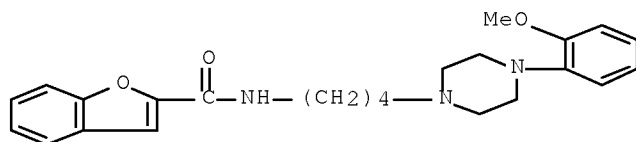
910127-41-2 910127-42-3 910127-43-4

RL: PAC (Pharmacological activity); PRP (Properties); BIOL (Biological study)

(CoMFA and CoMSIA investigations of dopamine D3 receptor ligands)

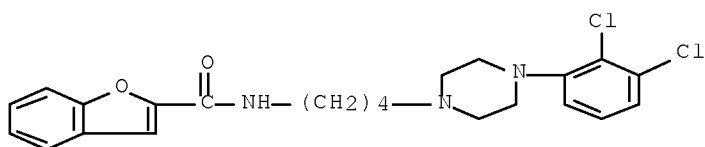
RN 474432-63-8 CAPLUS

CN 2-Benzofurancarboxamide, N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]-
(CA INDEX NAME)



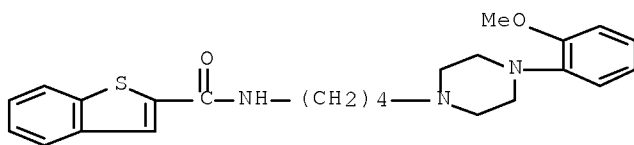
RN 474432-64-9 CAPLUS

CN 2-Benzofurancarboxamide, N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]-
(CA INDEX NAME)



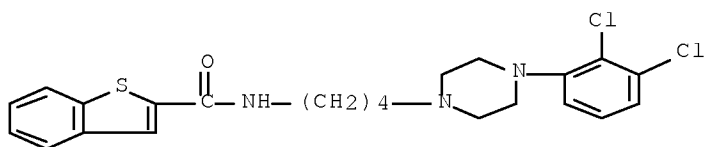
RN 474432-65-0 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



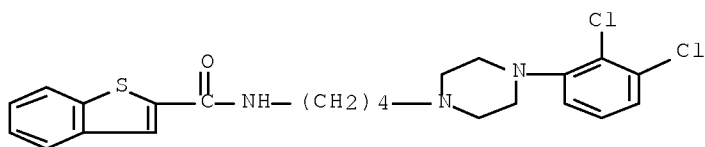
RN 474432-66-1 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



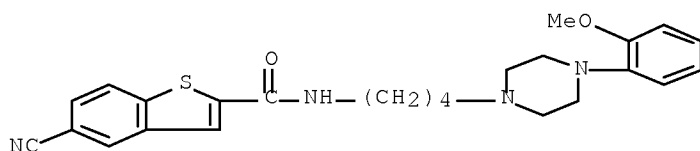
RN 474432-66-1 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



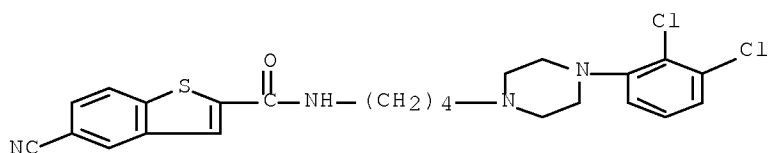
RN 644988-68-1 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, 5-cyano-N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



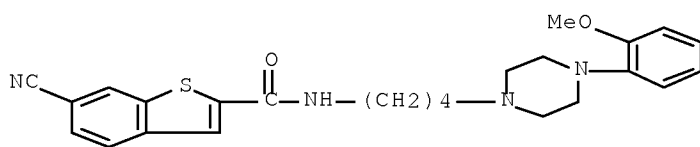
RN 644988-69-2 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, 5-cyano-N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



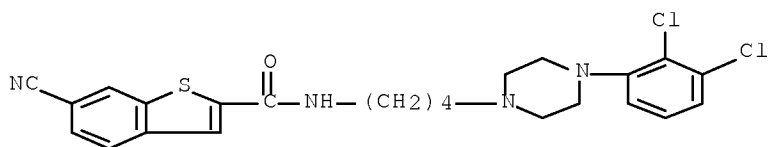
RN 644988-70-5 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, 6-cyano-N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



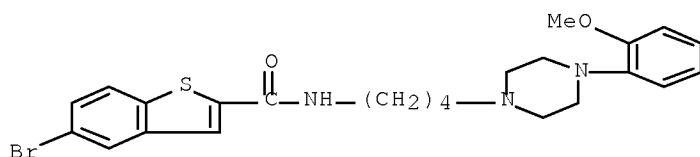
RN 644988-71-6 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, 6-cyano-N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



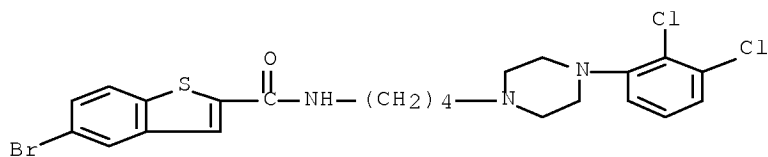
RN 644988-72-7 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, 5-bromo-N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



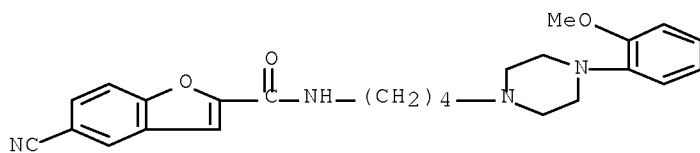
RN 644988-73-8 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, 5-bromo-N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



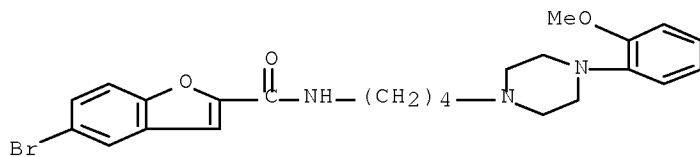
RN 644988-81-8 CAPLUS

CN 2-Benzofurancarboxamide, 5-cyano-N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



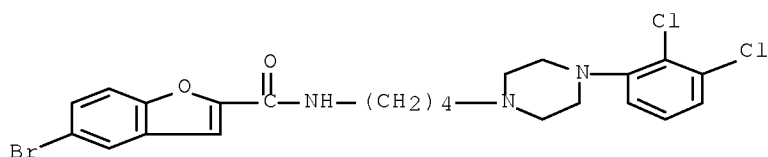
RN 644988-82-9 CAPLUS

CN 2-Benzofurancarboxamide, 5-bromo-N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



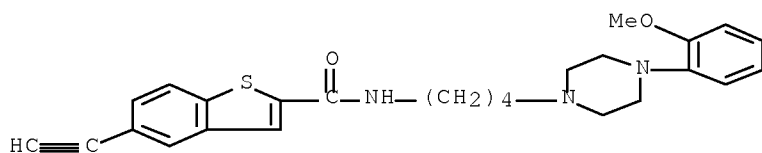
RN 644988-83-0 CAPLUS

CN 2-Benzofurancarboxamide, 5-bromo-N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



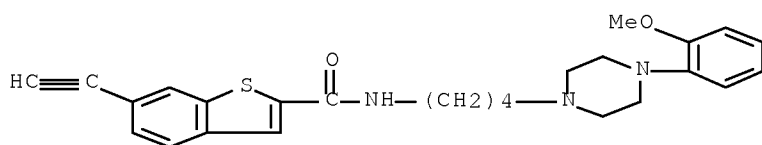
RN 910127-38-7 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, 5-ethynyl-N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



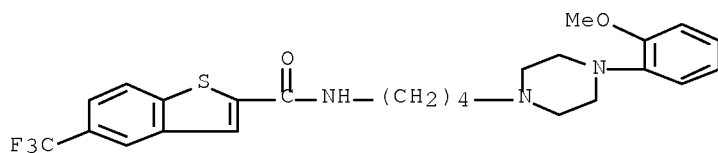
RN 910127-39-8 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, 6-ethynyl-N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



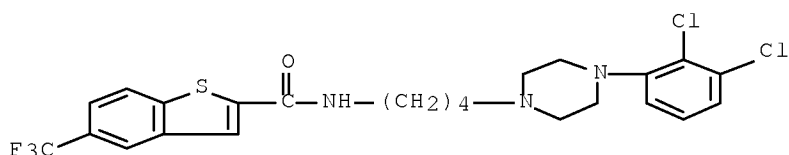
RN 910127-40-1 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]-5-(trifluoromethyl)- (CA INDEX NAME)



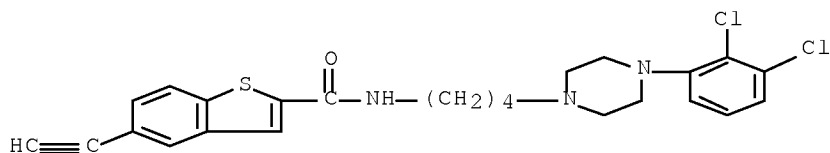
RN 910127-41-2 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]-5-(trifluoromethyl)- (CA INDEX NAME)



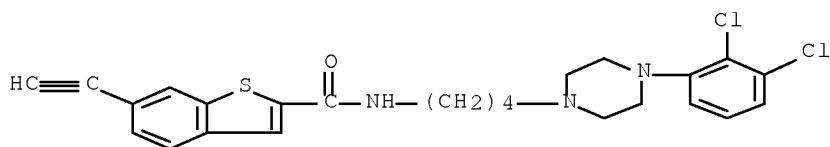
RN 910127-42-3 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]-5-ethynyl- (CA INDEX NAME)



RN 910127-43-4 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]-6-ethynyl- (CA INDEX NAME)



REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 31 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:685906 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 145:96764

TITLE: Dopamine D2 and D3 receptors in human putamen, caudate nucleus, and globus pallidus

AUTHOR(S): Seeman, Philip; Wilson, Alan; Gmeiner, Peter; Kapur, Shitij

CORPORATE SOURCE: Department of Pharmacology, University of Toronto, Toronto, ON, M5S 1A8, Can.

SOURCE: Synapse (Hoboken, NJ, United States) (2006), 60(3), 205-211

CODEN: SYNAET; ISSN: 0887-4476

PUBLISHER: Wiley-Liss, Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Because radioactive raclopride and radioactive (+)-4-propyl-9-hydroxynaphthoxazine ((+)-PHNO) are used to image dopamine (DA) D2 and D3 receptors in the striatum and globus pallidus in humans, the present study examined the proportions of D2 and D3 receptors in postmortem tissues from

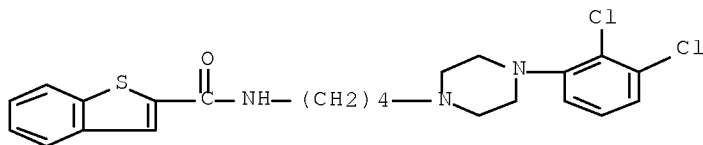
these regions. Conflicting results were obtained when using a single concentration of remoxipride to occlude D2 receptors or using a single concentration of U99194A or FAUC 365 to occlude D3 receptors. However, using a range of concns. of FAUC 365, a D3-selective antagonist, to inhibit the binding [3H]raclopride or [3H]-(+)-PHNO to D3 receptors at low concns. (1-10 nM) and to inhibit ligand binding to D2 receptors at higher concns. (100-2000 nM), it was possible to measure the proportion of D2 and D3 receptors in the tissues. This method revealed that these 2 radioligands detected only D2 receptors in the dorsal putamen and the dorsal caudate nucleus, but detected a mixed population of 67% D2 and 33% D3 DA receptors in the ventral putamen, ventral caudate, and globus pallidus. The present findings are in good agreement with the known gene expression data for D2 and D3 receptors in these human brain regions.

IT 474432-66-1, FAUC 365

RL: BSU (Biological study, unclassified); BIOL (Biological study)
(dopamine D2 and D3 receptors in human putamen, caudate nucleus, and globus pallidus)

RN 474432-66-1 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 31 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:681093 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 145:145751

TITLE: Preparation of arylpiperazine derivatives as modulators of dopamine and serotonin receptors for the treatment of neuropsychiatric disorders

INVENTOR(S): Campiani, Guiseppe; Butini, Stefania; Fattorusso, Caterina; Trotta, Francesco; Franceschini, Silvia; De Angelis, Meri; Nielsen, Karin Sandager

PATENT ASSIGNEE(S): Universita Degli Studi Di Siena, Italy

SOURCE: PCT Int. Appl., 94 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

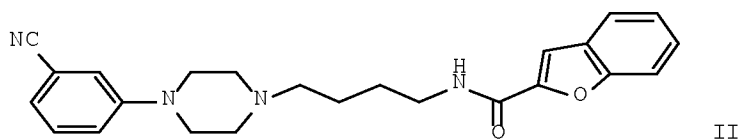
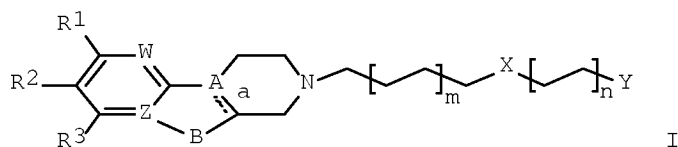
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006072608	A2	20060713	WO 2006-EP50001	20060102
WO 2006072608	A3	20060928		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE,

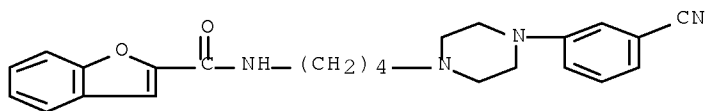
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 VN, YU, ZA, ZM, ZW
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 GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
 KG, KZ, MD, RU, TJ, TM
 AU 2006204522 A1 20060713 AU 2006-204522 20060102
 CA 2593266 A1 20060713 CA 2006-2593266 20060102
 EP 1836192 A2 20070926 EP 2006-700234 20060102
 R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
 IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR
 PRIORITY APPLN. INFO.: DK 2005-4 A 20050103
 US 2005-641006P P 20050104
 WO 2006-EP50001 W 20060102
 OTHER SOURCE(S): MARPAT 145:145751
 GI



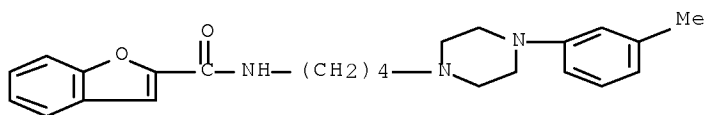
AB Title compds. I [wherein R1 - R3 = H, (cyclo)alkyl, alkoxy, etc.; A = CH or N when a = single bod; A = C when a = double bond; Z = CH or N when B = absent; Z = C when B = CH2, =CH- or NH; W = (un)substituted CH or N; m, n = 0-2; X= absent, O, S, etc.; Y = (un)substituted Ph, heteroaryl, heterocycllyl, etc.] or enantiomers, mixts. of enantiomers, pharmaceutically acceptable salts and N-oxides thereof, which are useful as modulators of dopamine and serotonin receptors, preferably the D3, D2-like and 5-HT2 receptor subtypes, and in particular useful for the treatment of neuropsychiatric disorders including schizophrenia (no data), were prepared For instance, successive DCC-mediated amidation of 2-benzofurancarboxylic acid with 4-amino-1-butanol (97% yield), bromination of the resultant alc. with CBr4/PPh3 (91% yield), and substitution with 1-(3-cyanophenyl)piperazine (preparation given) (90% yield) gave phenylpiperazine II.

IT 898532-77-9P 898532-85-9P 898533-12-5P
 898533-13-6P 898533-14-7P 898533-59-0P
 898533-60-3P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (drug candidate; preparation of arylpiperazine derivs. as modulators of dopamine and serotonin receptors for the treatment of neuropsychiatric disorders)
 RN 898532-77-9 CAPLUS

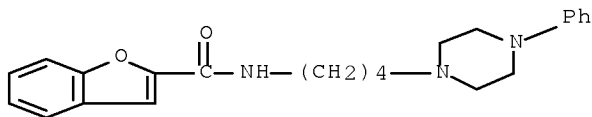
CN 2-Benzofurancarboxamide, N-[4-[4-(3-cyanophenyl)-1-piperazinyl]butyl]-
(CA INDEX NAME)



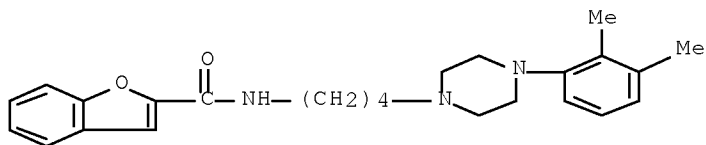
RN 898532-85-9 CAPLUS
CN 2-Benzofurancarboxamide, N-[4-[4-(3-methylphenyl)-1-piperazinyl]butyl]-
(CA INDEX NAME)



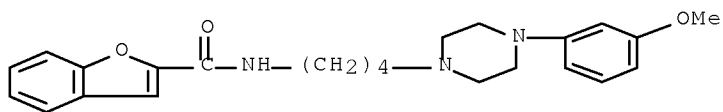
RN 898533-12-5 CAPLUS
CN 2-Benzofurancarboxamide, N-[4-(4-phenyl-1-piperazinyl)butyl]- (CA INDEX
NAME)



RN 898533-13-6 CAPLUS
CN 2-Benzofurancarboxamide, N-[4-[4-(2,3-dimethylphenyl)-1-piperazinyl]butyl]-
(CA INDEX NAME)

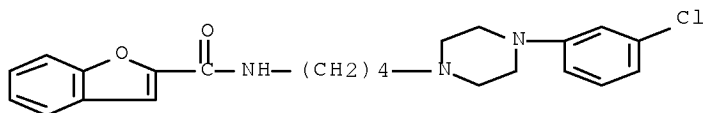


RN 898533-14-7 CAPLUS
CN 2-Benzofurancarboxamide, N-[4-[4-(3-methoxyphenyl)-1-piperazinyl]butyl]-
(CA INDEX NAME)



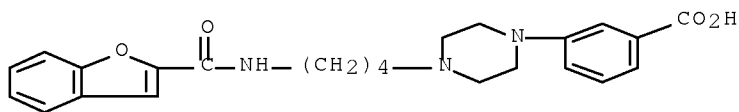
RN 898533-59-0 CAPLUS

CN 2-Benzofurancarboxamide, N-[4-[4-(3-chlorophenyl)-1-piperazinyl]butyl]-
(CA INDEX NAME)



RN 898533-60-3 CAPLUS

CN Benzoic acid, 3-[4-[4-[(2-benzofuranylcarbonyl)amino]butyl]-1-piperazinyl]-
(CA INDEX NAME)



L4 ANSWER 8 OF 31 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:476261 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 145:137258

TITLE: Fancy Bioisosteres: Novel Paracyclophane Derivatives

As Super-Affinity Dopamine D3 Receptor Antagonists

AUTHOR(S): Schlotter, Karin; Boeckler, Frank; Huebner, Harald;
Gmeiner, Peter

CORPORATE SOURCE: Department of Medicinal Chemistry, Emil Fischer
Center, Friedrich Alexander University, Erlangen,
D-91052, Germany

SOURCE: Journal of Medicinal Chemistry (2006), 49(12),
3628-3635

CODEN: JMCMAR; ISSN: 0022-2623

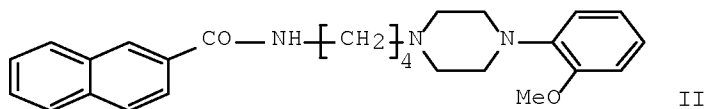
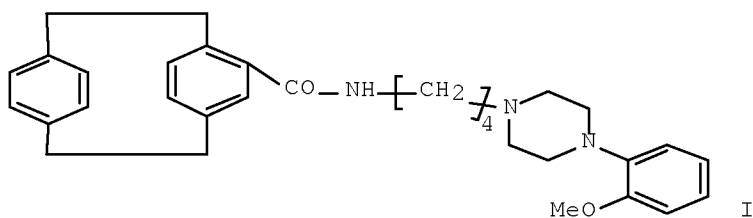
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 145:137258

GI



AB The exploration of the chemical diversity space depends on the discovery of novel bioisosteric elements. As a continuation of our project on bilayered arene surrogates, the authors herein report on [2.2]paracyclophane-derived dopamine D3 receptor antagonists of type 4 and 6. For the most promising test compound (I), bearing a 2-methoxyphenyl substituent, a stereocontrolled preparation was performed when the planar chirality of enantiomers (R)-I (FAUC 418) and (S)-I caused a considerable differentiation of D3 binding, which is indicated by K_i values of 0.19 and 3.0 nM, resp. Functional expts. showed D3 antagonist properties for the paracyclophane derivs. of type 6. To elucidate putative bioactive low-energy conformations, DFT-based studies including the calcn. of diagnostic magnetic shielding properties were performed. An 89% increase in volume for the [2.2]paracyclophane moiety compared to that of the monolayered benzofuran of lead compound (II) indicates higher plasticity of GPCR binding regions than usually expected.

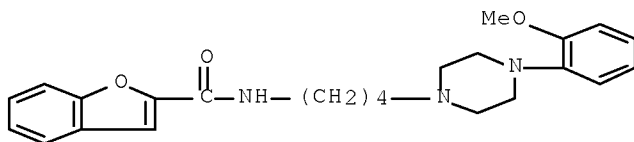
IT 474432-63-8

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(novel paracyclophane derivs. as super-affinity dopamine D3 receptor antagonists)

RN 474432-63-8 CAPLUS

CN 2-Benzofurancarboxamide, N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 31 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:109789 CAPLUS Full-text

DOCUMENT NUMBER: 144:324648

TITLE: Selective antagonist at D3 receptors, but not non-selective partial agonists, influences the expression of cocaine-induced conditioned place

preference in free-feeding rats
AUTHOR(S): Cervo, Luigi; Burbassi, Silvia; Colovic, Milena; Caccia, Silvio
CORPORATE SOURCE: Department of Neuroscience, Via Eritrea 62 Istituto di Ricerche, Istituto di Ricerche Farmacologiche "Mario Negri", Milan, 20157, Italy
SOURCE: Pharmacology, Biochemistry and Behavior (2005), 82(4), 727-734
CODEN: PBBHAU; ISSN: 0091-3057
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The non-selective dopamine (DA) D3 partial agonist BP 897 influenced rats' seeking behavior induced by cocaine-associated cues but there are contradictions about its ability to modulate cocaine-induced conditioned place preference (CPP), and mechanisms involved. We therefore re-evaluated its activity on both acquisition and expression of these behaviors, taking into consideration the actual brain concns. of unchanged drug and its potential active metabolite 1-(2-methoxyphenyl)-piperazine (oOCH3PP), as well as its neg. motivational properties. BP 897 induced conditioned place aversion (CPA) at 3 mg/kg, but not at 0.3 and 1 mg/kg. However, in this range of amply spaced doses BP 897 did not affect the acquisition and expression of cocaine (10 mg/kg i.p.) CPP in rats, although its brain concns. were well above those affecting in vitro D3 receptors. Concns. of oOCH3PP were below the limits of quantification of the anal. procedure. As concerns the expression behavior, its structurally and pharmacol. related derivative N-[4-[4-(2-methoxyphenyl)piperazin-1-yl]butyl]benzo[b]furan-2-carboxamide (1 and 3 mg/kg, i.p.) also had no such effect. By contrast, the selective D3 receptor antagonist SB-277011-A (3 mg/kg, i.p.) antagonized the expression of cocaine-induced CPP, supporting the suggestion that "full" antagonist activity at D3 receptors is necessary to prevent 10 mg/kg cocaine-induced place conditioning in free-feeding rats.

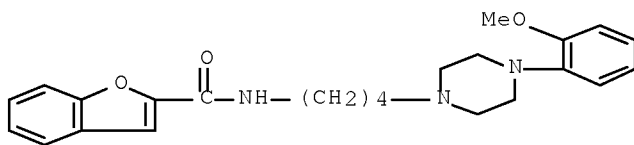
IT 474432-63-8

RL: BSU (Biological study, unclassified); PAC (Pharmacological activity);
BIOL (Biological study)

(selective antagonist at D3 receptors, but not non-selective partial agonists, influences the expression of cocaine-induced conditioned place preference in free-feeding rats)

RN 474432-63-8 CAPLUS

CN 2-Benzofuran-2-carboxamide, N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]-
(CA INDEX NAME)



REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

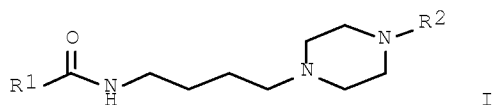
L4 ANSWER 10 OF 31 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:1247836 CAPLUS Full-text

DOCUMENT NUMBER: 144:128936

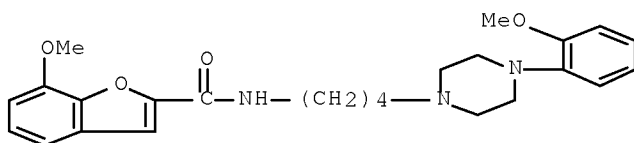
TITLE: Design, Synthesis, and Binding Affinities of Potential Positron Emission Tomography (PET) Ligands for

AUTHOR(S): Visualization of Brain Dopamine D3 Receptors
 Leopoldo, Marcello; Lacivita, Enza; De Giorgio, Paola;
 Colabufo, Nicola A.; Niso, Mauro; Berardi, Francesco;
 Perrone, Roberto
 CORPORATE SOURCE: Dipartimento Farmaco-Chimico, Universita degli Studi
 di Bari, Bari, 70125, Italy
 SOURCE: Journal of Medicinal Chemistry (2006), 49(1), 358-365
 CODEN: JMCMAR; ISSN: 0022-2623
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 144:128936
 GI

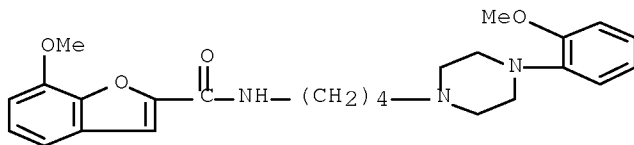


AB The synthesis of compds. I [R1 = 7-methoxybenzofuran-2-yl, quinoxalin-6-yl, 3-(2-pyrimidyl)phenyl, 5-(2-furyl)-3-pyrazolyl, etc.; R2 = 2-MeOC6H4, 2-benzimidazolyl, 5-methoxy-2-benzisoxazolyl, etc.], structurally related to the high-affinity dopamine D3 receptor ligand N-[4-[4-(2,3-dichlorophenyl)piperazin-1-yl]butyl]-7-methoxy-2-benzofurancarboxamide (II), is reported. All compds. were specifically designed as potential PET radioligands for brain D3 receptors visualization, having lipophilicity within a range for high brain uptake and weak nonspecific binding ($2 < \text{ClogP} < 3.5$) and bearing a methoxy substituent for easy access to labeling with the positron emitter isotope ^{11}C . I [R1 = 4-(4-morpholinyl)phenyl, 4-(1-imidazolyl)phenyl, 5-(2-furyl)-3-pyrazolyl; R2 = 5-methoxy-2-benzisoxazolyl] displayed good D3 receptor affinities (K_i values 38.0, 22.6, and 21.3 nM, resp.) and were selective over D2 receptor. Moreover, these compds. were able to permeate the Caco-2 cell monolayer, differently from compound II. Although the goal to identify potential PET radioligands with subnanomolar affinities for D3 receptor was not achieved, the proposed strategy could be a starting point for future developments.

IT 873662-57-8P
 RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (preparation, lipophilicity and brain dopamine D3 receptor binding affinities of N-(arylpiperazinyl)butyl heteroarylcarboxamides as potential positron emission tomog. ligands)
 RN 873662-57-8 CAPLUS
 CN 2-Benzofurancarboxamide, 7-methoxy-N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



IT 873662-81-8P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (preparation, lipophilicity and brain dopamine D3 receptor binding affinities of N-(arylpiperazinyl)butyl heteroarylcarboxamides as potential positron emission tomog. ligands)
 RN 873662-81-8 CAPLUS
 CN 2-Benzofurancarboxamide, 7-methoxy-N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]-, dihydrochloride (9CI) (CA INDEX NAME)



● 2 HCl

REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 31 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:1059039 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 143:477941

TITLE: 11C-Labeling of N-[4-[4-(2,3-Dichlorophenyl)piperazin-1-yl]butyl]arylcarboxamide Derivatives and Evaluation as Potential Radioligands for PET Imaging of Dopamine D3 Receptors

AUTHOR(S): Turolla, Elia A.; Matarrese, Mario; Belloli, Sara; Moresco, Rosa M.; Simonelli, Pasquale; Todde, Sergio; Fazio, Ferruccio; Magni, Fulvio; Kienle, Marzia Galli; Leopoldo, Marcello; Berardi, Francesco; Colabufo, Nicola A.; Lacivita, Enza; Perrone, Roberto

CORPORATE SOURCE: Institute of Molecular Bioimaging and Physiology-CNR, Milan, 20132, Italy

SOURCE: Journal of Medicinal Chemistry (2005), 48(22), 7018-7023

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 143:477941

AB The selective dopamine D3 receptor ligands N-4-[4-[(2,3-dichlorophenyl)piperazin-1-yl]butyl]-1-methoxy-2-naphthalenecarboxamide (I) and N-4-[4-[(2,3-dichlorophenyl)piperazin-1-yl]butyl]-7-methoxy-2-benzofurancarboxamide (II) were labeled with 11C (t1/2 = 20.4 min) as potential radioligands for the non-invasive assessment of the dopamine D3 neurotransmission system in vivo with positron emission tomog. (PET). The radiosynthesis consisted in an O-methylation of the desmethyl precursors N-[4-[4-(2,3-dichlorophenyl)piperazin-1-yl]butyl]-1-hydroxy-2-naphthalenecarboxamide and N-[4-[4-(2,3-dichlorophenyl)piperazin-1-yl]butyl]-7-hydroxy-2-benzofurancarboxamide with [11C]methyl iodide using tert-BuOK/HMPA

and KOH/DMSO, resp. The radiotracers [11C]1 and [11C]2 were obtained in 35 min with over 99% radiochem. purity, 74 ± 37 GBq/ μ mol of specific radioactivity, 13% and 26% radiochem. yield (EOB, decay-corrected). Distribution studies in rats demonstrated that the new tracers [11C]-I and [11C]-II cross the blood-brain barrier and localize in the brain. However, the kinetics of cerebral uptake did not reflect the regional expression of the D3 receptors. Despite their in vitro pharmacol. profile, [11C]-I and [11C]-II do not display an in vivo behavior suitable to image D3 receptor expression using PET.

IT 869664-21-1P

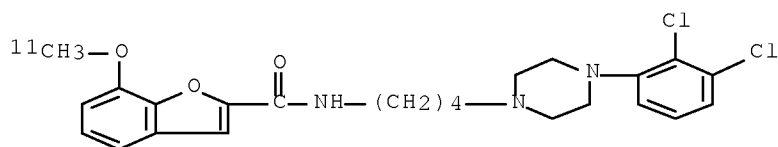
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation);

BIOL (Biological study); PREP (Preparation)

(preparation of 11C-labeled N-[[[(dichlorophenyl)piperazinyl]butyl](methoxy)benzofurancarboxamide and study of its applicability as radioligand for PET imaging of dopamine D3 receptors)

RN 869664-21-1 CAPLUS

CN 2-Benzofurancarboxamide, N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]-7-(methoxy-11C)- (9CI) (CA INDEX NAME)



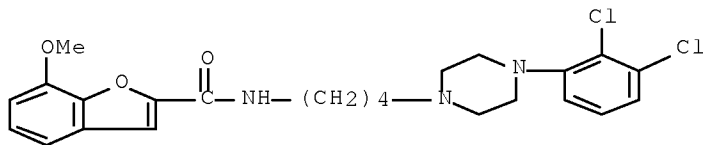
IT 687634-09-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of 11C-labeled N-[[[(dichlorophenyl)piperazinyl]butyl](methoxy)benzofurancarboxamide and study of its applicability as radioligand for PET imaging of dopamine D3 receptors)

RN 687634-09-9 CAPLUS

CN 2-Benzofurancarboxamide, N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]-7-methoxy- (CA INDEX NAME)



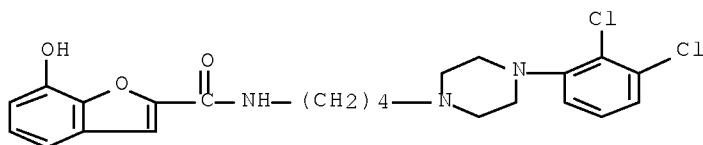
IT 869664-17-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 11C-labeled N-[[[(dichlorophenyl)piperazinyl]butyl]arylcarboxamide derivs. and study of their applicability as radioligands for PET imaging of dopamine D3 receptors)

RN 869664-17-5 CAPLUS

CN 2-Benzofurancarboxamide, N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]-7-hydroxy- (CA INDEX NAME)



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 12 OF 31 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:607838 CAPLUS Full-text

DOCUMENT NUMBER: 143:259488

TITLE: Predicting dopamine receptors binding affinity of N-[4-(4-arylpiperazin-1-yl) butyl]aryl carboxamides: Computational approach using topological descriptors

AUTHOR(S): Lather, Viney; Madan, A. K.

CORPORATE SOURCE: Faculty of Pharmaceutical Sciences, M. D. University, Rohtak, 124001, India

SOURCE: Current Drug Discovery Technologies (2005), 2(2), 115-121

CODEN: CDDTAF; ISSN: 1570-1638

PUBLISHER: Bentham Science Publishers Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Relation between the topol. indexes and Dopamine D3 and D4 receptor binding affinities of N-[4-(4-Arylpiperazin-1-yl)butyl]aryl carboxamides has been investigated. Three topol. indexes, the Wiener's Index- a distance-based topol. descriptor, mol. connectivity index- an adjacency based topol. descriptor and eccentric connectivity index- an adjacency-cum-distance based topol. descriptor were used for the present investigations. A data set comprising of 37 substituted N-[4-(4-Arylpiperazin-1-yl)butyl]aryl carboxamides was selected for the present studies. The values of the Wiener's index, eccentric connectivity index and mol. connectivity index for each of the 37 analogs comprising the data set were computed using inhouse computer program. Resultant data was subsequently analyzed and suitable models were developed after identification of active ranges. Subsequently, a biol. activity was assigned to each analog using these models, which was then compared with the reported D3 and D4 receptor binding affinity. These models exhibited exceptionally high predictability.

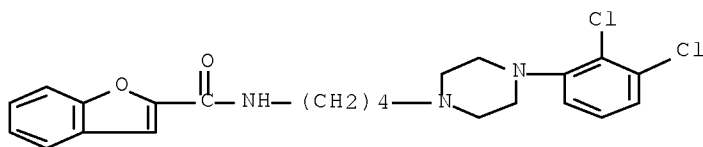
IT 474432-64-9 474432-66-1 687634-09-9

RL: PAC (Pharmacological activity); PRP (Properties); BIOL (Biological study)

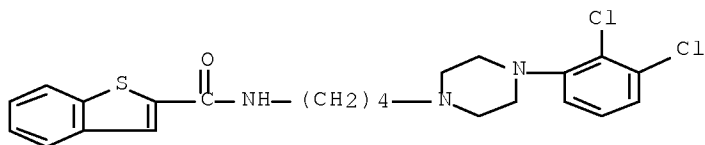
(predicting dopamine receptors binding affinity of aryl carboxamides)

RN 474432-64-9 CAPLUS

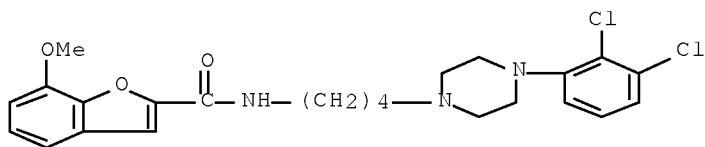
CN 2-Benzofurancarboxamide, N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



RN 474432-66-1 CAPLUS
 CN Benzo[b]thiophene-2-carboxamide, N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)

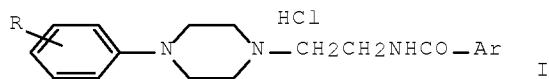


RN 687634-09-9 CAPLUS
 CN 2-Benzofurancarboxamide, N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]-7-methoxy- (CA INDEX NAME)



REFERENCE COUNT: 63 THERE ARE 63 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 13 OF 31 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2005:510486 CAPLUS Full-text
 DOCUMENT NUMBER: 143:193972
 TITLE: Pharmacophore-based design, synthesis, biological evaluation, and 3D-QSAR studies of aryl-piperazines as α 1-adrenoceptor antagonists
 AUTHOR(S): Li, Min-Yong; Fang, Hao; Xia, Lin
 CORPORATE SOURCE: Department of Medicinal Chemistry, China Pharmaceutical University, Nanjing, 210009, Peop. Rep. China
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(13), 3216-3219
 CODEN: BMCLE8; ISSN: 0960-894X
 PUBLISHER: Elsevier B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 143:193972
 GI

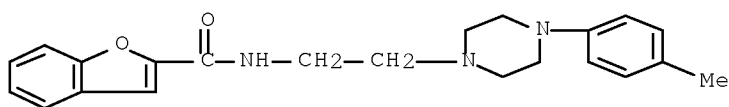


AB Aryl-piperazine amides I (R = 2,4-di-Me, 5-chloro-2-methoxy, 3-methoxy, 4-methoxy, 2-methoxy, 4-Me, 2,4-di-Me, 2-methoxy; Ar = 4-pyridinyl, 2-furanyl, 3-coumarinyl, 3-pyridinyl, 2-benzofuranyl) were designed based on pharmacophore for uro-selective $\alpha 1$ -adrenoceptor antagonists, synthesized and examined for biol. activity. Within this series, I (R = 5-chloro-2-methoxy, Ar = 2-furanyl; R = 3-methoxy, Ar = 2-furanyl; R = 2-methoxy, Ar = 2-furanyl) showed similar or better $\alpha 1$ -adrenoceptor antagonistic activity compared with prazosin. The 3D-QSAR study of these compds. may provide useful information for the development of novel aryl-piperazines as uro-selective $\alpha 1$ -adrenoceptor antagonists, which can be used for the treatment of benign prostatic hyperplasia (BPH) with fewer side effects.

IT 861903-43-7P 861903-46-0P 861903-53-9P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (preparation and biol. activity of aryl-piperazines as $\alpha 1$ -adrenoceptor antagonists)

RN 861903-43-7 CAPLUS

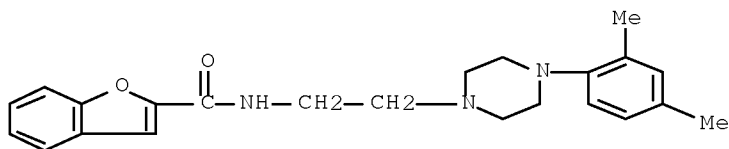
CN 2-Benzofurancarboxamide, N-[2-[4-(4-methylphenyl)-1-piperazinyl]ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 861903-46-0 CAPLUS

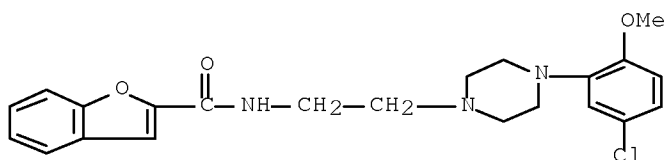
CN 2-Benzofurancarboxamide, N-[2-[4-(2,4-dimethylphenyl)-1-piperazinyl]ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 861903-53-9 CAPLUS

CN 2-Benzofurancarboxamide, N-[2-[4-(5-chloro-2-methoxyphenyl)-1-piperazinyl]ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 14 OF 31 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:31512 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 142:190237

TITLE: Novel Heterocyclic Trans Olefin Analogues of N-{4-[4-(2,3-Dichlorophenyl)piperazin-1-yl]butyl}arylcarboxamides as Selective Probes with High Affinity for the Dopamine D3 Receptor

AUTHOR(S): Grundt, Peter; Carlson, Erin E.; Cao, Jianjing; Bennett, Christina J.; McElveen, Elizabeth; Taylor, Michelle; Luedtke, Robert R.; Newman, Amy Hauck

CORPORATE SOURCE: Medicinal Chemistry Section National Institute on Drug Abuse-Intramural Research Program, National Institutes of Health, Baltimore, MD, 21224, USA

SOURCE: Journal of Medicinal Chemistry (2005), 48(3), 839-848
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 142:190237

AB Dopamine D3 receptor subtypes have been hypothesized to play a pivotal role in modulating the reinforcing and drug-seeking effects induced by cocaine. However, definitive pharmacol. investigations have been hampered by the lack of highly D3 receptor selective compds. that can be used in vivo. To address this problem, the potent and D3-receptor-selective antagonist NGB 2904 (1, 9H-fluorene-2-carboxylic acid {4-[(2,3- dichlorophenyl)-piperazin-1-yl]-butyl}-amide, K_i (hD3) = 2.0 nM, K_i (hD2L) = 112 nM, D2/D3 selectivity ratio of 56) was chosen as a lead structure for chemical modification in an attempt to reduce its high lipophilicity (c log D = 6.94) while optimizing D3 receptor binding affinity and D2/D3 selectivity. A series of >30 novel analogs were synthesized, and their binding affinities were evaluated in competition binding assays in HEK 293 cells transfected with either D2L, D3, or D4 human dopamine receptors using the high affinity, selective D2-like receptor antagonist 125I-IABN. Structural diversity in the aryl amide end of the mol. was found to have a major influence on (sub)nanomolar D3 receptor affinity and D2/D3 selectivity, which was optimized using a more rigid trans-butenyl linker between the aryl amide and the piperazine. Several analogs demonstrated superior D3 receptor binding affinities and selectivities as compared to the parent ligand. Compound 29 (N-{4-[4-(2,3-dichlorophenyl)-piperazin-1-yl]-trans-but-2-enyl}-4-pyridine-2-yl-benzamide) displayed the most promising pharmacol. profile (K_i (hD3) = 0.7 nM, K_i (hD2L) = 93.3 nM, D2/D3 selectivity ratio of 133). In addition, this ligand inhibited quinpirole stimulation of mitogenesis at human dopamine D3 receptors transfected into Chinese hamster ovary (CHO) cells, with an EC50 value of 3.0 nM. Compound 29 was a nearly 5 times more potent antagonist at the D3 receptor than 1 (EC50 = 14.4 nM).

Moreover, a decrease in c log D value of .apprx.2 orders of magnitude was determined for this novel D3-receptor-preferring ligand, compared to 1. In summary, chemical modification of 1 has resulted in compds. with high affinity and selectivity for D3 receptors. The most promising candidate, compound 29, is currently being evaluated in animal models of cocaine abuse and will provide an important tool with which to elucidate the role of D3 receptors in drug reinforcement in vivo.

IT 675599-59-4P 675599-61-8P

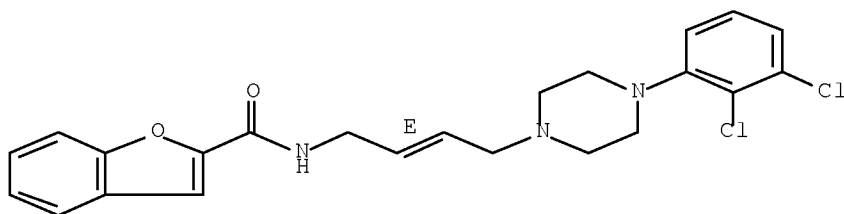
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(N-{4-[4-(2,3-Dichlorophenyl)piperazin-1-yl]butyl}arylcarboxamide
derivs.: preparation and affinity for D3 receptor)

RN 675599-59-4 CAPLUS

CN 2-Benzofurancarboxamide, N-[(2E)-4-[4-(2,3-dichlorophenyl)-1-piperazinyl]-2-butenyl]-, monohydrochloride (9CI) (CA INDEX NAME)

Double bond geometry as shown.



● HCl

RN 675599-61-8 CAPLUS

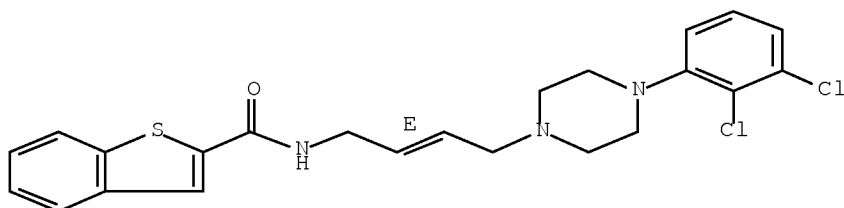
CN Benzo[b]thiophene-2-carboxamide, N-[(2E)-4-[4-(2,3-dichlorophenyl)-1-piperazinyl]-2-butenyl]-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 675599-60-7

CMF C23 H23 Cl2 N3 O S

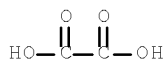
Double bond geometry as shown.



CM 2

CRN 144-62-7

CMF C2 H2 O4



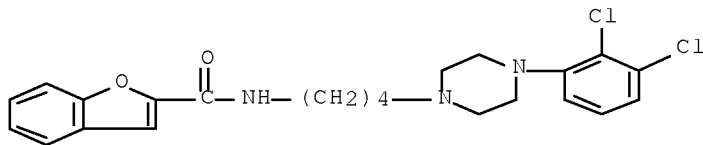
IT 474432-64-9 474432-66-1

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
(Biological study); USES (Uses)

(N-{4-[4-(2,3-Dichlorophenyl)piperazin-1-yl]butyl}arylcarboxamide
derivs.: preparation and affinity for D3 receptor)

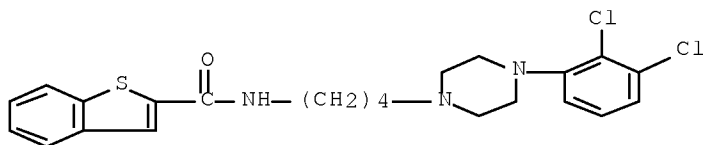
RN 474432-64-9 CAPLUS

CN 2-Benzofurancarboxamide, N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]-
(CA INDEX NAME)



RN 474432-66-1 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, N-[4-[4-(2,3-dichlorophenyl)-1-
piperazinyl]butyl]- (CA INDEX NAME)



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 15 OF 31 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:23570 CAPLUS Full-text

DOCUMENT NUMBER: 142:254418

TITLE: Modeling the Similarity and Divergence of Dopamine
D2-like Receptors and Identification of Validated
Ligand-Receptor Complexes

AUTHOR(S): Boeckler, Frank; Lanig, Harald; Gmeiner, Peter

CORPORATE SOURCE: Department of Medicinal Chemistry, Emil Fischer,
Friedrich-Alexander University, Erlangen, D-91052,
Germany

SOURCE: Journal of Medicinal Chemistry (2005), 48(3), 694-709
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

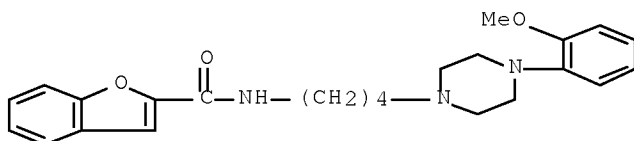
AB Focusing on the similarity and divergence of GPCR subtypes and their ligand interactions, we generated dopamine D2, D3, and D4 receptor models based on the rhodopsin crystal structure and refined these with an extensive MM/MD protocol. After validation by diagnostic exptl. data, subtype-specific relative positions of TM1, 2, 6, and 7 and bending angles of TM7 were found. To sample the conformational space of the complex, we performed simulated-annealing runs of the receptor protein with the sub-nanomolar antagonist spiperone. Docking a representative set of ligands, we were able to identify one superior model for each subtype when excellent correlations between predicted energies of binding and exptl. affinities ($r^2 = 0.72$ for D2, 0.91 for D3 and 0.77 for D4) could be observed. Further anal. revealed general ligand interactions with ASP3.32 and aromatic residues in TM6/7 and individual key interactions with TM1 and TM2 residues of the D3 and D4 receptor models, resp.

IT 474432-63-8 474432-66-1, Fauc 365

RL: BSU (Biological study, unclassified); BIOL (Biological study)
(modeling the similarity and divergence of dopamine D2-like receptors
and identification of validated ligand-receptor complexes)

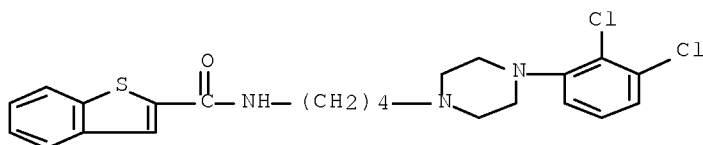
RN 474432-63-8 CAPLUS

CN 2-Benzofurancarboxamide, N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]-
(CA INDEX NAME)



RN 474432-66-1 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



REFERENCE COUNT: 77 THERE ARE 77 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 16 OF 31 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:17188 CAPLUS Full-text

DOCUMENT NUMBER: 142:348097

TITLE: Predicting dopamine D3 receptor binding affinity of
N-(ω -(4-(2-methoxyphenyl)piperazin-1-
yl)alkyl)carboxamides: Computational approach using
topological descriptors

AUTHOR(S): Lather, Viney; Madan, Anil Kumar

CORPORATE SOURCE: Faculty of Pharmaceutical Sciences, M. D. University,

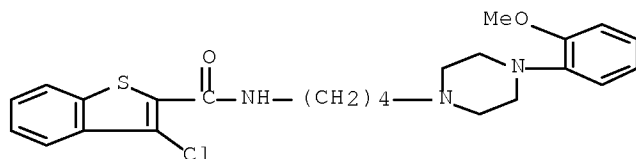
SOURCE: Rohtak, 124001, India
MATCH (2004), 52, 65-89
CODEN: MATCDY; ISSN: 0340-6253
PUBLISHER: University of Kragujevac, Faculty of Science
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Relationship between the topol. indexes and Dopamine D3 receptor binding affinity of N-(ω -(4-(2-Methoxyphenyl)piperazin-1-yl)alkyl)carboxamides has been investigated. Three topol. indexes - the Wiener's Index- a distance-based topol. descriptor, Zagreb group parameter- an adjacency based topol. descriptor and eccentric connectivity index- an adjacency-cum-distance based topol. descriptor were used for the present investigations. A data set comprising of 73 differently substituted N-(ω -(4-(2-Methoxyphenyl)piperazin-1-yl)alkyl)carboxamides was selected for the present studies. The values of the Wiener's index, Zagreb group parameter and eccentric connectivity index for each of the 73 analogs. Comprising the data set were computed using an in house computer program. Resultant data was subsequently analyzed and suitable models were developed after identification of active ranges. Subsequently, a biol. activity was assigned to each analog using these models, which was then compared with the reported Dopamine D3 receptor binding affinity. The degree of predictability of these models was found to vary from a min. of 82% to a maximum of 86%.

IT 560117-00-2
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(relationship between the topol. indexes and dopamine D3 receptor binding affinity of N-(ω -(4-(2-methoxyphenyl)piperazin-1-yl)alkyl)carboxamides using computational approach)

RN 560117-00-2 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, 3-chloro-N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 17 OF 31 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:1043345 CAPLUS Full-text
DOCUMENT NUMBER: 142:106556
TITLE: Synthesis and in vitro binding of N-phenyl piperazine analogs as potential dopamine D3 receptor ligands
AUTHOR(S): Chu, Wenhua; Tu, Zhude; McElveen, Elizabeth; Xu, Jinbin; Taylor, Michelle; Luedtke, Robert R.; Mach, Robert H.
CORPORATE SOURCE: Department of Radiology, Division of Radiological Sciences, Washington University School of Medicine, St. Louis, MO, 63110, USA
SOURCE: Bioorganic & Medicinal Chemistry (2004), Volume Date 2005, 13(1), 77-87

CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 142:106556

AB A series of N-(2-methoxyphenyl)piperazine and N-(2,3-dichlorophenyl)piperazine analogs were prepared and their affinities for dopamine D₂, D₃, and D₄ receptors were measured in vitro. Binding studies were also conducted to determine if the compds. bound to sigma (σ_1 and σ_2) and serotonin (5-HT_{1A}, 5-HT_{2A}, 5-HT_{2B}, 5-HT_{2C}, 5-HT₃, 5-HT₄, 5-HT₅, 5-HT₆, and 5-HT₇) receptors. The results of the current study revealed a number of compds. (12b, 12c, 12e, and 12g) having a high affinity for D₃ (K_i at D₃ receptors ranging from 0.3 to 0.9 nM) vs. D₂ (K_i at D₂ receptors ranging from 40 to 53 nM) receptors and a log P value indicating that they should readily cross the blood brain barrier (log P = 2.6-3.5). All of the compds. evaluated in this study had a high affinity for serotonin 5-HT_{1A} receptors. These compds. may be useful as probes for studying the behavioral pharmacol. of the dopamine D₃ receptor, as well as lead compds. for the development of radiotracers for studying D₃ receptor regulation in vivo with the functional imaging technique, positron emission tomog.

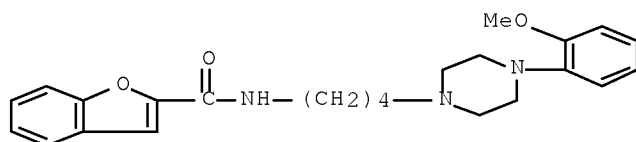
IT 474432-63-8P 474432-64-9P 474432-65-0P

RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(synthesis and in vitro binding of N-Ph piperazine analogs as potential dopamine D₃ receptor ligands)

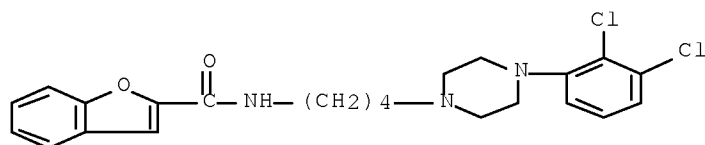
RN 474432-63-8 CAPLUS

CN 2-Benzofurancarboxamide, N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]-
(CA INDEX NAME)



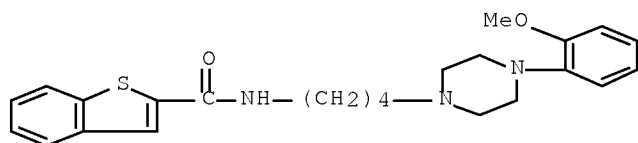
RN 474432-64-9 CAPLUS

CN 2-Benzofurancarboxamide, N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]-
(CA INDEX NAME)



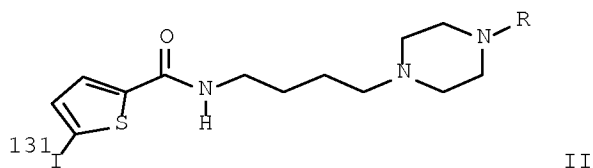
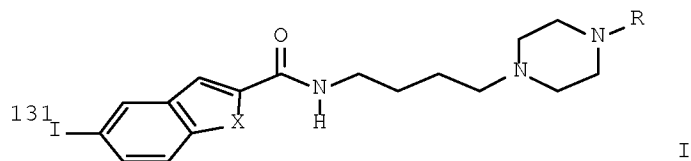
RN 474432-65-0 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 18 OF 31 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2004:523292 CAPLUS Full-text
 DOCUMENT NUMBER: 141:207172
 TITLE: Synthesis and radioiodination of selective ligands for the dopamine D3 receptor subtype
 AUTHOR(S): Hocke, Carsten; Prante, Olaf; Lober, Stefan; Hubner, Harald; Gmeiner, Peter; Kuwert, Torsten
 CORPORATE SOURCE: Department of Nuclear Medicine, Erlangen, D-91054, Germany
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(15), 3963-3966
 CODEN: BMCLE8; ISSN: 0960-894X
 PUBLISHER: Elsevier Science B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 141:207172
 GI



AB A series of radioiodinated heteroaryl carboxamides I (X = O, S; R = 2-MeOC₆H₄, 2,3-Cl₂C₆H₃) and II, the potential imaging agents for the D3 receptor by single-photon emission tomog. (SPET), has been synthesized in high radiochem. yields (53-85%) and revealed high affinity and selectivity for the dopamine D3 receptor. Binding data showed a 15-560-fold selectivity for the dopamine D3 over D2. A 2,3-dichloro substitution pattern on the phenylpiperazine moiety led to the highest subtype selectivity, whereas the 2-methoxy substituted compds. showed superior D3 affinity.
 IT 744213-81-8P 744213-82-9P 744213-83-0P
 744213-84-1P 817162-44-0P 817162-54-2P

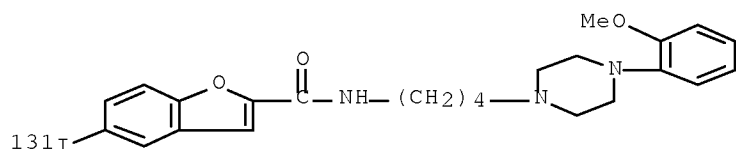
817162-55-3P 817162-56-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL
(Biological study); PREP (Preparation)

(preparation of radioiodinated N-piperazinylbutyl heteroaryl carboxamides as
selective ligands for the dopamine D3 receptor subtype)

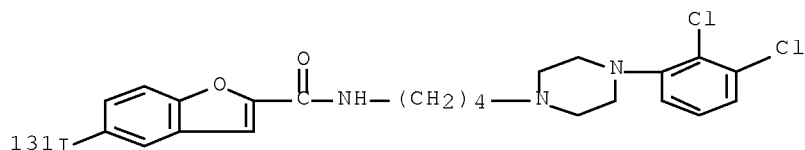
RN 744213-81-8 CAPLUS

CN 2-Benzofurancarboxamide, 5-(iodo-¹³¹I)-N-[4-[4-(2-methoxyphenyl)-1-
piperazinyl]butyl]- (9CI) (CA INDEX NAME)



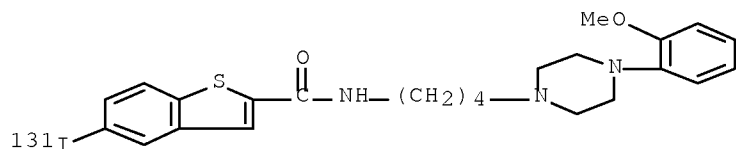
RN 744213-82-9 CAPLUS

CN 2-Benzofurancarboxamide, N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]-
5-(iodo-¹³¹I)- (9CI) (CA INDEX NAME)



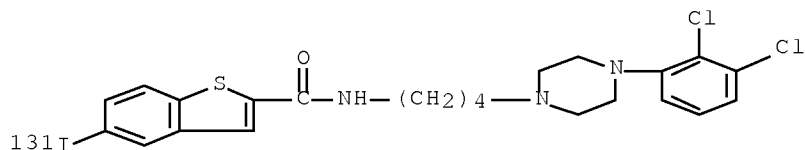
RN 744213-83-0 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, 5-(iodo-¹³¹I)-N-[4-[4-(2-methoxyphenyl)-1-
piperazinyl]butyl]- (9CI) (CA INDEX NAME)



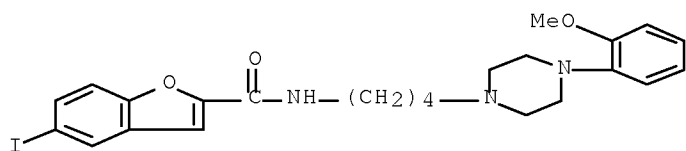
RN 744213-84-1 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, N-[4-[4-(2,3-dichlorophenyl)-1-
piperazinyl]butyl]-5-(iodo-¹³¹I)- (9CI) (CA INDEX NAME)



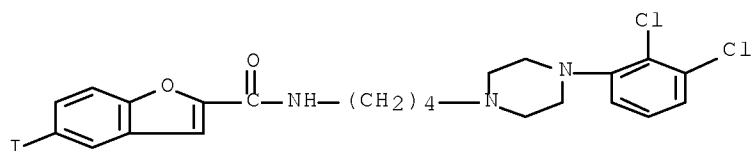
RN 817162-44-0 CAPLUS

CN 2-Benzofurancarboxamide, 5-iodo-N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



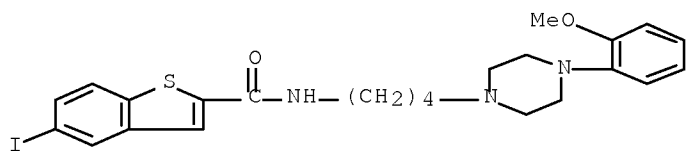
RN 817162-54-2 CAPLUS

CN 2-Benzofurancarboxamide, N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]-5-iodo- (CA INDEX NAME)



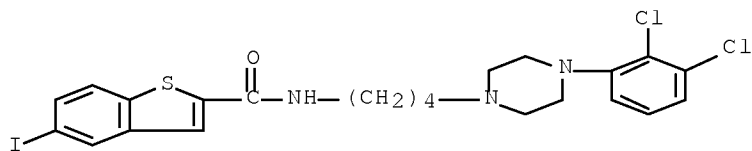
RN 817162-55-3 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, 5-iodo-N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



RN 817162-56-4 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]-5-iodo- (CA INDEX NAME)



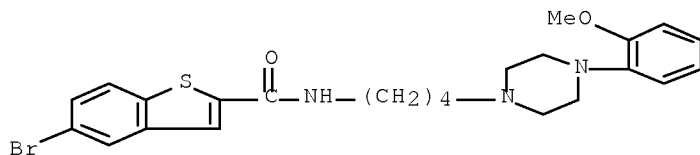
IT 644988-72-7P 644988-73-8P 644988-82-9P
644988-83-0P 744213-75-0P 744213-76-1P
744213-77-2P 744213-78-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(preparation of radioiodinated N-piperazinylbutyl heteroaryl carboxamides as
selective ligands for the dopamine D3 receptor subtype)

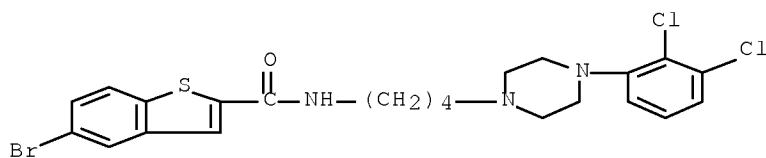
RN 644988-72-7 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, 5-bromo-N-[4-[4-(2-methoxyphenyl)-1-
piperazinyl]butyl]- (CA INDEX NAME)



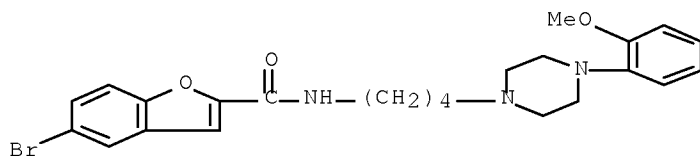
RN 644988-73-8 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, 5-bromo-N-[4-[4-(2,3-dichlorophenyl)-1-
piperazinyl]butyl]- (CA INDEX NAME)



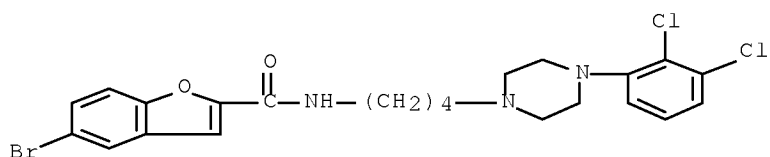
RN 644988-82-9 CAPLUS

CN 2-Benzofurancarboxamide, 5-bromo-N-[4-[4-(2-methoxyphenyl)-1-
piperazinyl]butyl]- (CA INDEX NAME)



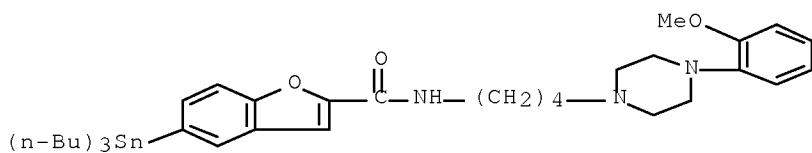
RN 644988-83-0 CAPLUS

CN 2-Benzofurancarboxamide, 5-bromo-N-[4-[4-(2,3-dichlorophenyl)-1-
piperazinyl]butyl]- (CA INDEX NAME)



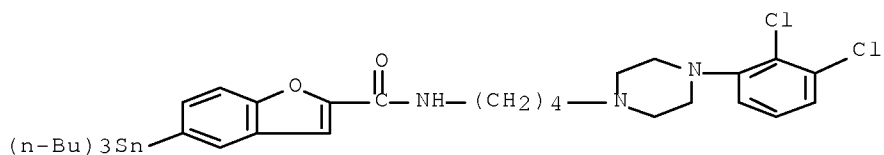
RN 744213-75-0 CAPLUS

CN 2-Benzofurancarboxamide, N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]-5-(tributylstannyl)- (CA INDEX NAME)



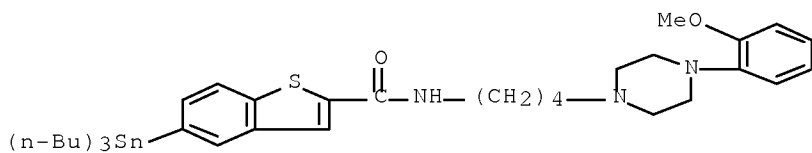
RN 744213-76-1 CAPLUS

CN 2-Benzofurancarboxamide, N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]-5-(tributylstannyl)- (CA INDEX NAME)



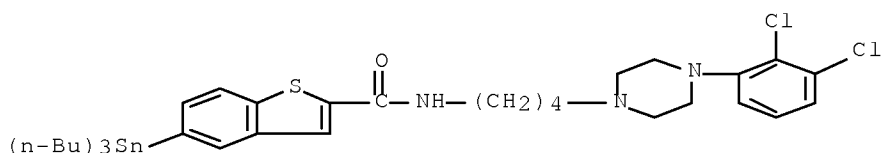
RN 744213-77-2 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]-5-(tributylstannyl)- (CA INDEX NAME)



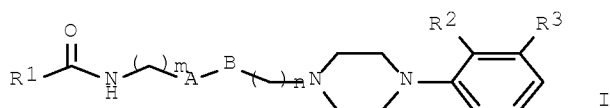
RN 744213-78-3 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]-5-(tributylstannyl)- (CA INDEX NAME)



L4 ANSWER 19 OF 31 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2004:252605 CAPLUS Full-text
 DOCUMENT NUMBER: 140:287411
 TITLE: Preparation of structurally rigid arylpiperazines as
 dopamine D3 receptor selective ligands
 INVENTOR(S): Newman, Amy; Grundt, Peter; Luedtke, Robert R.
 PATENT ASSIGNEE(S): United States Department of Health and Human Services,
 USA
 SOURCE: PCT Int. Appl., 34 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004024878	A2	20040325	WO 2003-US28895	20030915
WO 2004024878	A3	20040701		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG CA 2498936 A1 20040325 CA 2003-2498936 20030915 AU 2003267201 A1 20040430 AU 2003-267201 20030915 US 2006106030 A1 20060518 US 2005-527594 20051213 PRIORITY APPLN. INFO.: US 2002-410715P P 20020914 WO 2003-US28895 W 20030915 OTHER SOURCE(S): MARPAT 140:287411 GI				



AB Title compds. [I; A = CH:CH, C.tplbond.C, cyclohexylene; B = null, CH:CH; R1 =
 (substituted) Ph, heteroaryl; R2 = H, halo, alkoxy; R3 = H, halo], were

prepared Thus, carbonyldiimidazole was stirred 1 h with 4-hydroxybenzoic acid in pyridine; 4-[4-(2,3-dichlorophenyl)piperazin-1-yl]but-2-enylamine (preparation given) in CHCl₃ was added followed by stirring overnight to give 51% N-[4-[4-(2,3-dichlorophenyl)piperazin-1-yl]but-2-enyl]-4-hydroxybenzamide (PG01015). PG01015 bound to cloned human D₃ receptors in HEK cells with 34-fold greater affinity than to D₂ receptors.

IT 675599-59-4 675599-61-8

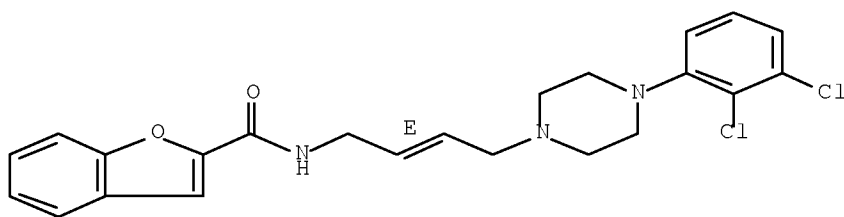
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(preparation of structurally rigid arylpiperazines as dopamine D₃ receptor selective ligands)

RN 675599-59-4 CAPLUS

CN 2-Benzofurancarboxamide, N-[(2E)-4-[4-(2,3-dichlorophenyl)-1-piperazinyl]-2-butenyl]-, monohydrochloride (9CI) (CA INDEX NAME)

Double bond geometry as shown.



● HCl

RN 675599-61-8 CAPLUS

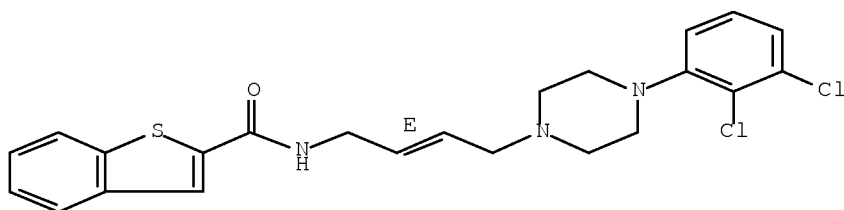
CN Benzo[b]thiophene-2-carboxamide, N-[(2E)-4-[4-(2,3-dichlorophenyl)-1-piperazinyl]-2-butenyl]-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 675599-60-7

CMF C23 H23 Cl2 N3 O S

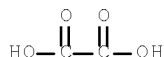
Double bond geometry as shown.



CM 2

CRN 144-62-7

CMF C2 H2 O4



L4 ANSWER 20 OF 31 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:41278 CAPLUS Full-text

DOCUMENT NUMBER: 140:94065

TITLE: Preparation of arylpiperazinylbutylheteroarenecarboxamides and related compounds as dopamine D3 ligands for the treatment of central nervous system diseases

INVENTOR(S): Gmeiner, Peter; Huebner, Harald; Schlotter, Karin

PATENT ASSIGNEE(S): Friedrich-Alexander-Universitaet Erlangen-Nuernberg, Germany

SOURCE: PCT Int. Appl., 56 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

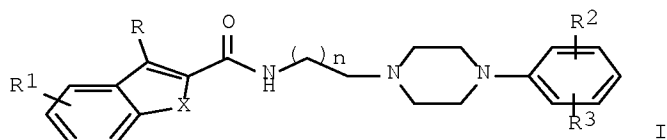
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004004729	A1	20040115	WO 2003-EP7060	20030702
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
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CA 2489396	A1	20040115	CA 2003-2489396	20030702
AU 2003246356	A1	20040123	AU 2003-246356	20030702
EP 1519726	A1	20050406	EP 2003-762588	20030702
EP 1519726	B1	20070221		
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CN 1665503	A	20050907	CN 2003-815742	20030702
JP 2005538974	T	20051222	JP 2004-518667	20030702
EP 1733727	A1	20061220	EP 2006-20274	20030702
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ES 2280799	T3	20070916	ES 2003-762588	20030702
ZA 2004010292	A	20051006	ZA 2004-10292	20041221
MX 2005PA00033	A	20050408	MX 2005-PA33	20050103
NO 2005000386	A	20050125	NO 2005-386	20050125
US 2005197343	A1	20050908	US 2005-519487	20050427
HK 1074579	A1	20070622	HK 2005-106891	20050810
PRIORITY APPLN. INFO.:			DE 2002-10230062	A 20020704

DE 2002-10232020 A 20020710
 EP 2003-762588 A3 20030702
 WO 2003-EP7060 W 20030702

OTHER SOURCE(S): MARPAT 140:94065
 GI



AB Title compds., e.g. [I; n = 1-4; R = H, alkyl, halo; (a) X = S, O; if R1 = OH, alkoxy, alkenyl, alkynyl, aryl, acyl, alkoxy carbonyl, cyano, then R2, R3 = H, OH, alkoxy, alkyl, alkenyl, alkynyl, aryl, halo, CF3, acyl, alkoxy carbonyl, cyano; or if R1 = H, alkyl, halo, CF3, then R2 = OH, alkenyl, alkynyl, aryl, acyl, alkoxy carbonyl, cyano, and R3 = H, OH, alkoxy, alkyl, alkenyl, alkynyl, aryl, halo, CF3, acyl, alkoxy carbonyl, cyano; (b) X = NH; R1 = H, OH, alkyl, alkoxy, alkenyl, alkynyl, aryl, CF3, acyl, alkoxy carbonyl, halo, cyano; R2, R3 = H, OH, alkoxy, alkyl, alkenyl, alkynyl, aryl, halo, CF3, acyl, alkoxy carbonyl, cyano; (c) X = Te; R1 = H, OH, alkyl, alkoxy, alkenyl, alkynyl, aryl, halo, CF3, acyl, alkoxy carbonyl, cyano; R2, R3 = H, OH, alkoxy, alkyl, alkenyl, alkynyl, aryl, halo, CF3, acyl, alkoxy carbonyl, cyano; the alkyl, alkenyl, alkynyl, and aryl groups may be substituted; with provisos], were prepared Thus, benzothiophene-2-carboxylic acid was heated with SOCl2 in PhMe/CHCl3/DMF at 90° to give a residue which in CHCl3 was added to 4-[4-(2-methoxyphenyl)piperazin-1-yl]butylamine and Et3N in CHCl3 followed by stirring for 15 h to give 68% N-[4-[4-(2-methoxyphenyl)piperazin-1-yl]butyl]-2-benzo[b]thiophenylcarboxamide. The latter showed partial agonist activity at D3 receptors with EC50 = 0.38 nM.

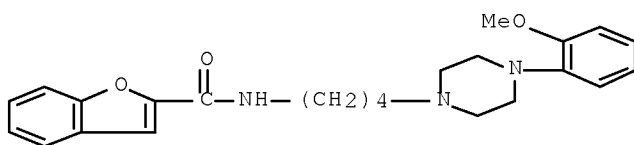
IT 474432-63-8P 474432-64-9P 474432-65-0P
 474432-66-1P 644988-68-1P 644988-69-2P
 644988-70-5P 644988-71-6P 644988-72-7P
 644988-73-8P 644988-81-8P 644988-82-9P
 644988-83-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of arylpiperazinylbutylheteroarenecarboxamides and related compds. as dopamine D3 ligands for the treatment of central nervous system diseases)

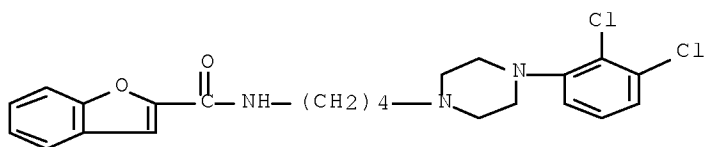
RN 474432-63-8 CAPLUS

CN 2-Benzofurancarboxamide, N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



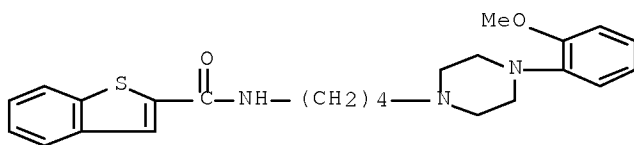
RN 474432-64-9 CAPLUS

CN 2-Benzofurancarboxamide, N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]-
(CA INDEX NAME)



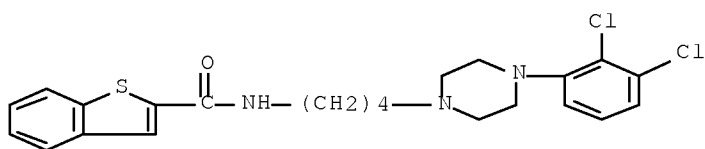
RN 474432-65-0 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



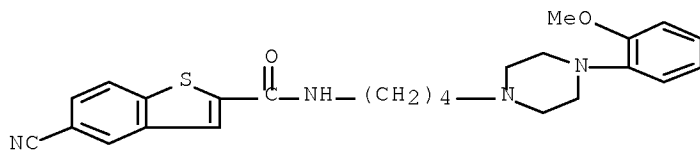
RN 474432-66-1 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



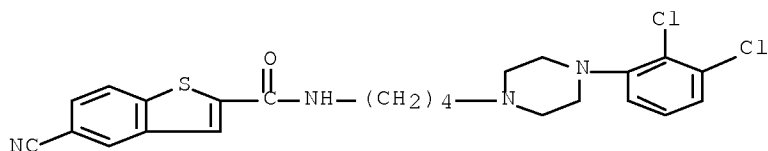
RN 644988-68-1 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, 5-cyano-N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



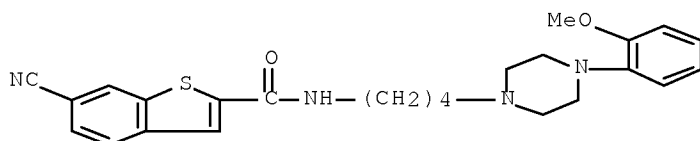
RN 644988-69-2 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, 5-cyano-N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



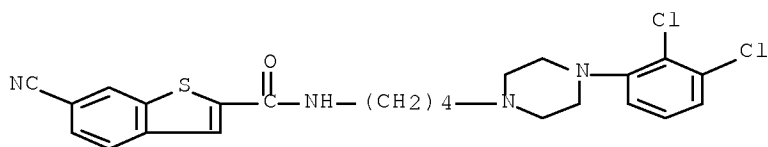
RN 644988-70-5 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, 6-cyano-N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



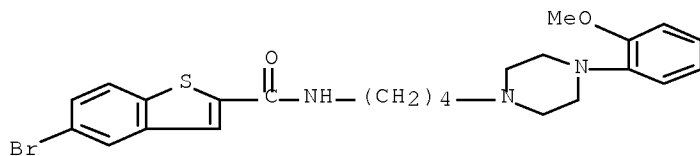
RN 644988-71-6 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, 6-cyano-N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



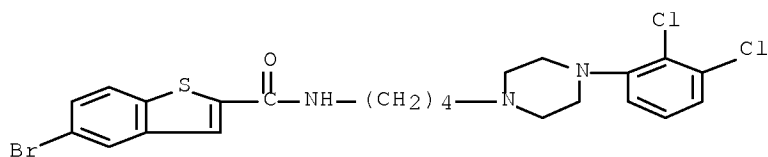
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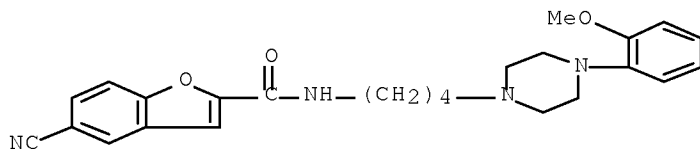
RN 644988-73-8 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, 5-bromo-N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



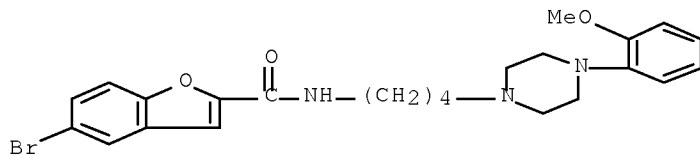
RN 644988-81-8 CAPLUS

CN 2-Benzofurancarboxamide, 5-cyano-N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



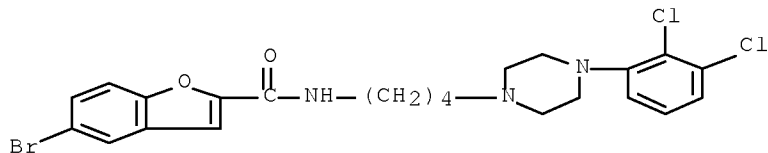
RN 644988-82-9 CAPLUS

CN 2-Benzofurancarboxamide, 5-bromo-N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



RN 644988-83-0 CAPLUS

CN 2-Benzofurancarboxamide, 5-bromo-N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



REFERENCE COUNT:

7

THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 21 OF 31 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:981477 CAPLUS [Full-text](#)

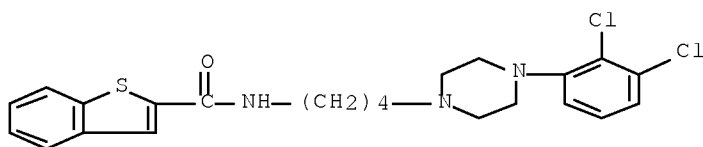
DOCUMENT NUMBER: 140:246107
 TITLE: Conformationally-flexible benzamide analogues as dopamine D3 and σ 2 receptor ligands
 AUTHOR(S): Mach, Robert H.; Huang, Yunsheng; Freeman, Rebekah A.; Wu, Li; Vangveravong, Suwanna; Luedtke, Robert R.
 CORPORATE SOURCE: PET Center, Department of Radiology, Wake Forest University School of Medicine, Winston-Salem, NC, 27157, USA
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(1), 195-202
 CODEN: BMCLE8; ISSN: 0960-894X
 PUBLISHER: Elsevier Science B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 140:246107

AB A series of conformationally-flexible analogs was prepared and their affinities for D2-like dopamine (D2, D3 and D4) were determined using in vitro radioligand binding assays. The results of this structure-activity relationship study identified one compound that bound with high affinity (K_i value=2 nM) and moderate selectivity (30-fold) for D3 compared to D2 receptors. In addition, this series of compds. were also tested for affinity at σ 1 and σ 2 receptors. We evaluated the affinity of these dopaminergic compds. at sigma receptors because (a) several antipsychotic drugs, which are high affinity antagonists at dopamine D2-like receptors, also bind to sigma receptors and (b) sigma receptors are expressed ubiquitously and at high levels (picomoles per mg proteins). It was observed that a number of analogs displayed high affinity and excellent selectivity for σ 2 vs. σ 1 receptors. Consequently, these novel compds. may be useful for characterizing the functional role of σ 2 receptors and for imaging the σ 2 receptor status of tumors in vivo with PET.

IT 474432-66-1
 RL: BSU (Biological study, unclassified); BIOL (Biological study) (conformationally-flexible benzamide analogs as dopamine D3 and σ 2 receptor ligands)

RN 474432-66-1 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



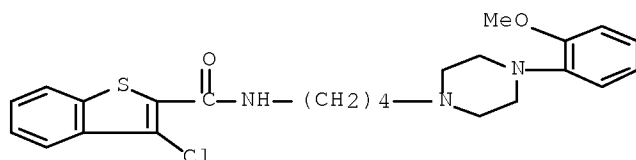
REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 22 OF 31 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2003:580003 CAPLUS Full-text
 DOCUMENT NUMBER: 139:111076
 TITLE: N-(ω -(4-(2-Methoxyphenyl)piperazin-1-yl)alkyl)carboxamides as Dopamine D2 and D3 Receptor Ligands
 AUTHOR(S): Hackling, Anneke; Ghosh, Robin; Perachon, Sylvie; Mann, Andre; Hoeltje, Hans-Dieter; Wermuth, Camille

G.; Schwartz, Jean-Charles; Sippl, Wolfgang; Sokoloff, Pierre; Stark, Holger
 CORPORATE SOURCE: Institut fuer Pharmazeutische Chemie, Johann Wolfgang Goethe-Universitaet, Frankfurt/Main, 60439, Germany
 SOURCE: Journal of Medicinal Chemistry (2003), 46(18), 3883-3899
 CODEN: JMCMAR; ISSN: 0022-2623
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 139:111076

AB The dopamine D3 receptor is recognized as a potential therapeutic target for the treatment of various neurol. and psychiatric disorders. Targetting high affinity and D3 vs. D2 receptor-preferring ligands, the partial agonist BP 897 was taken as a lead structure. Variations in the spacer and the aryl moiety led to N-alkylated 1-(2-methoxyphenyl)piperazines with markedly improved affinity and selectivity. Mol. modeling studies supported the structural development. Pharmacophore models for dopamine D2 and D3 receptor ligands were developed from their potentially bioactive conformation and were compared in order to get insight into mol. properties of importance for D2/D3 receptor selectivity. For the 72 compds. presented here, an extended and more linear conformation in the aliphatic or aryl spacers turned out to be crucial for dopamine D3 receptor selectivity. Structural diversity in the aryl moiety (benzamides, heteroarylamides, arylimides) had a major influence on (sub)nanomolar D3 receptor affinity, which was optimized with more rigid aryl acrylamide derivs. Compound 38 (ST 280, (E)-4-iodo-N-(4-(4-(2-methoxyphenyl)piperazin-1-yl)butyl)cinnamoylamide) displayed a most promising pharmacol. profile (K_i (hD3) = 0.5 nM; K_i (hD2L) = 76.4 nM; selectivity ratio of 153), and above that, compound 38 offered the prospect of a novel radioligand as a pharmacol. tool for various D3 receptor-related in vitro and in vivo investigation.

IT 560117-00-2P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (synthesis and structure-activity relationship of N-(4-(2-methoxyphenyl)piperazin-1-yl)alkyl)carboxamides as dopamine D2 and D3 receptor ligands)
 RN 560117-00-2 CAPLUS
 CN Benzo[b]thiophene-2-carboxamide, 3-chloro-N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



REFERENCE COUNT: 64 THERE ARE 64 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 23 OF 31 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2003:576171 CAPLUS Full-text
 DOCUMENT NUMBER: 139:261251

TITLE: Synthesis and Pharmacological Evaluation of Potent and Highly Selective D3 Receptor Ligands: Inhibition of Cocaine-Seeking Behavior and the Role of Dopamine D3/D2 Receptors

AUTHOR(S): Campiani, Giuseppe; Butini, Stefania; Trotta, Francesco; Fattorusso, Caterina; Catalanotti, Bruno; Aiello, Francesca; Gemma, Sandra; Nacci, Vito; Novellino, Ettore; Stark, Jennifer Ann; Cagnotto, Alfredo; Fumagalli, Elena; Carnovali, Francesco; Cervo, Luigi; Mennini, Tiziana

CORPORATE SOURCE: Dipartimento Farmaco Chimico Tecnologico, Universita di Siena, Siena, 53100, Italy

SOURCE: Journal of Medicinal Chemistry (2003), 46(18), 3822-3839
CODEN: JMCMAR; ISSN: 0022-2623

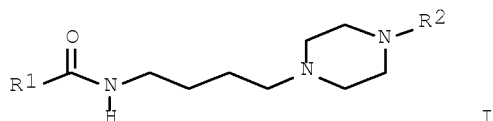
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:261251

GI



AB The synthesis, pharmacol. evaluation, and structure-activity relationships (SARs) of a series of novel arylalkyl piperazines, e.g. I (R1 = quinolin-2-yl, quinoxalin-2-yl, 2-indolyl, benzofuran-2-yl, isoquinolin-3-yl, etc.; R2 = 2-MeOC6H4, 4-NCC6H4, 2,4-Cl2C6H3, 3,4-Cl2C6H3), are described. In binding studies, the new derivs. were tested against a panel of dopamine, serotonin, and noradrenaline receptor subtypes. Focusing mainly on dopamine D3 receptors, SAR studies brought to light a number of structural features required for high receptor affinity and selectivity. The intrinsic pharmacol. properties of a subset of potent D3 receptor ligands were also assessed in [35S]-GTPγS binding assays. Evidence from animal studies, in particular, has highlighted the dopaminergic system's role in how environmental stimuli induce drug-seeking behavior. Introduction of an indole ring linked to a dichlorophenylpiperazine system provided two of the most potent and selective ligands known to date (D3 receptor affinity in the picomolar range), which were therefore tested in vivo for their effect in the cocaine-seeking behavior induced by reintroduction of cocaine-associated stimuli after a long period of abstinence, and without any further cocaine. I (R1 = benzofuran-2-yl; R2 = 2-MeOC6H4), a nonselective partial D3 receptor agonist with a pharmacol. profile similar to BP897, and I (R1 = 2-indolyl; R2 = 2,4-Cl2C6H3), a potent and selective D3 antagonist, reduced the number of active lever presses induced by reintroduction of cocaine-associated stimuli. However, I (R1 = 5-chloro-2-indolyl; R2 = 2,4-Cl2C6H3), a highly potent and selective D3 partial agonist, did not have any effect on cocaine-seeking behavior. Although brain uptake studies are needed to establish whether these compds. achieve brain concns. comparable to those active in vitro on the D3 receptor, our expts. suggest that antagonism at D2 receptors might significantly contribute to the reduction of cocaine craving by partial D3 agonists.

IT 474432-63-8P 600710-10-9P 600710-11-0P

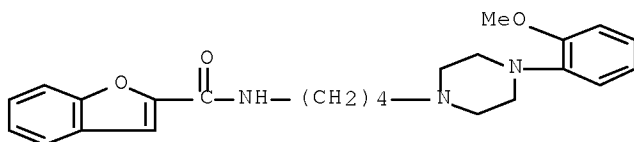
600710-13-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL
(Biological study); PREP (Preparation)

(preparation of heteroarylalkyl arylpiperazines as selective D3 receptor
ligands for inhibition of cocaine-seeking behavior)

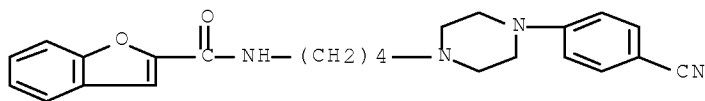
RN 474432-63-8 CAPLUS

CN 2-Benzofurancarboxamide, N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]-
(CA INDEX NAME)



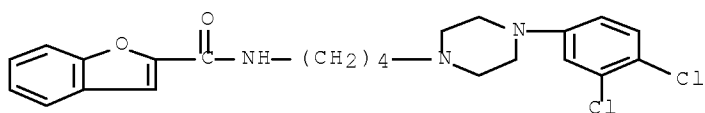
RN 600710-10-9 CAPLUS

CN 2-Benzofurancarboxamide, N-[4-[4-(4-cyanophenyl)-1-piperazinyl]butyl]-
(CA INDEX NAME)



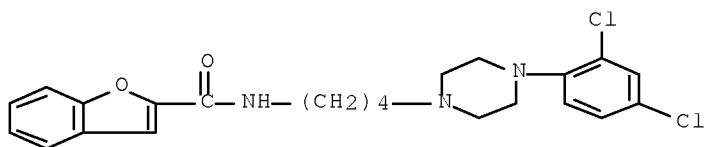
RN 600710-11-0 CAPLUS

CN 2-Benzofurancarboxamide, N-[4-[4-(3,4-dichlorophenyl)-1-piperazinyl]butyl]-
(CA INDEX NAME)



RN 600710-13-2 CAPLUS

CN 2-Benzofurancarboxamide, N-[4-[4-(2,4-dichlorophenyl)-1-piperazinyl]butyl]-
(CA INDEX NAME)



REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 24 OF 31 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:884258 CAPLUS Full-text

DOCUMENT NUMBER: 138:100350

TITLE: Structure-Affinity Relationship Study on
N-[4-(4-Arylpiperazin-1-yl)butyl]arylcarboxamides as
Potent and Selective Dopamine D3 Receptor Ligands

AUTHOR(S): Leopoldo, Marcello; Berardi, Francesco; Colabufo,
Nicola A.; De Giorgio, Paola; Lacivita, Enza; Perrone,
Roberto; Tortorella, Vincenzo

CORPORATE SOURCE: Dipartimento Farmaco-Chimico, Universita degli Studi
di Bari, Bari, 70126, Italy

SOURCE: Journal of Medicinal Chemistry (2002), 45(26),
5727-5735

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:100350

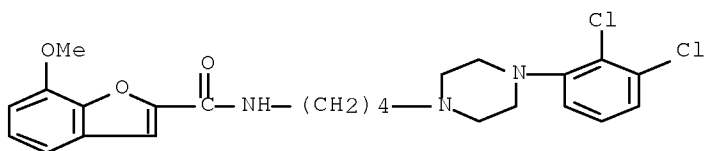
AB The benzamide PB12 (N-[2-[4-(4-chlorophenyl)piperazin-1-yl]ethyl]-3-methoxybenzamide) (1), already reported as potent and selective dopamine D4 receptor ligand, has been modified searching for structural features that could lead to D3 receptor affinity. Changes in the aromatic ring linked to N-1 piperazine ring led to the identification of 2-methoxyphenyl and 2,3-dichlorophenyl derivs. (compds. 6 and 13) displaying moderate D3 affinity (K_i = 145 and 31 nM, resp.). Intermediate alkyl chain elongation in compds. 1, 6, and 13 improved binding affinity for the D3 receptor and decreased the D4 affinity (compds. 18-26). Among these latter compds., the N-[4-[4-(2,3-dichlorophenyl)piperazin-1-yl]butyl]-3-methoxybenzamide (19) was further modified with the replacement of the 2,3-dichlorophenyl moiety (compds. 27-30) or of the 3-methoxyphenyl ring (compds. 31-41). In this way, we identified several high-affinity D3 ligands ($0.13 \text{ nM} < K_i$'s $< 4.97 \text{ nM}$) endowed with high selectivity over D2, D4, 5-HT_{1A}, and α_1 receptors. In addition, N-[4-[4-(2,3-dimethylphenyl)piperazin-1-yl]butyl]-3-methoxybenzamide (27) and N-[4-[4-(2,3-dichlorophenyl)piperazin-1-yl]butyl]-7-methoxy-2-benzofurancarboxamide (41) appear to be valuable candidates for positron emission tomog. (PET) because of their affinity values, lipophilicity properties, and liability of ¹¹C labeling in the O-Me position.

IT 486393-36-6P

RL: DGN (Diagnostic use); PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and structure-affinity relationship of N-[4-(4-Arylpiperazin-1-yl)butyl]arylcarboxamides as potent and selective D3 receptor ligands)

RN 486393-36-6 CAPLUS

CN 2-Benzofurancarboxamide, N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]-7-methoxy-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

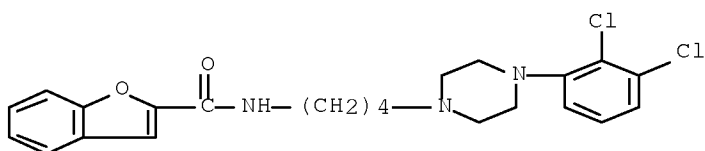
IT 486393-31-1P 486393-35-5P

RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation and structure-affinity relationship of N-[4-(4-Arylpiperazin-1-yl)butyl]arylcarboxamides as potent and selective D3 receptor ligands)

RN 486393-31-1 CAPLUS

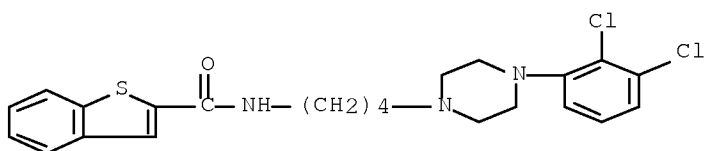
CN 2-Benzofurancarboxamide, N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 486393-35-5 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]-, monohydrochloride (9CI) (CA INDEX NAME)

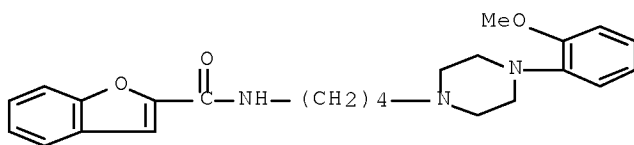


● HCl

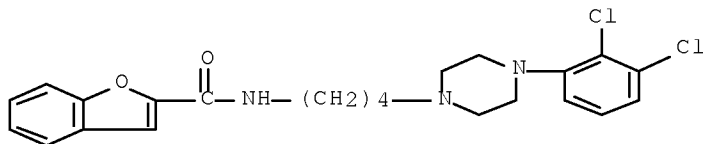
REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 25 OF 31 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2002:669886 CAPLUS [Full-text](#)
 DOCUMENT NUMBER: 137:345606

TITLE: Interactive SAR Studies: Rational Discovery of Super-Potent and Highly Selective Dopamine D3 Receptor Antagonists and Partial Agonists
 AUTHOR(S): Bettinetti, Laura; Schlotter, Karin; Huebner, Harald; Gmeiner, Peter
 CORPORATE SOURCE: Department of Medicinal Chemistry, Emil Fischer Center, Friedrich-Alexander University, Erlangen, D-91052, Germany
 SOURCE: Journal of Medicinal Chemistry (2002), 45(21), 4594-4597
 CODEN: JMCMAR; ISSN: 0022-2623
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 137:345606
 AB Starting from dopamine receptor ligand BP897, an interactive drug discovery process leading to heterocyclic bioisosteres is demonstrated. The four step strategy involved a careful optimization of geometric and electronic properties by systematic modification of the attachment points and heteroatoms, resp. Efficacy tuning by modification of the Ph substituents led to both D3 partial agonists and full antagonists. The benzothiophenes FAUC346 and FAUC365 revealed outstanding D3 affinity and subtype selectivity.
 IT 474432-63-8P 474432-64-9P 474432-65-0P
 474432-66-1P
 RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (rational discovery of super-potent and highly selective dopamine D3 receptor antagonists and partial agonists)
 RN 474432-63-8 CAPLUS
 CN 2-Benzofurancarboxamide, N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]-(CA INDEX NAME)

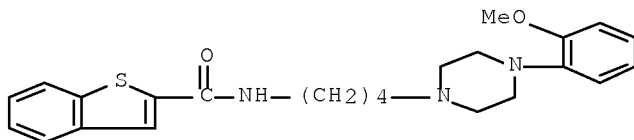


RN 474432-64-9 CAPLUS
 CN 2-Benzofurancarboxamide, N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]-(CA INDEX NAME)



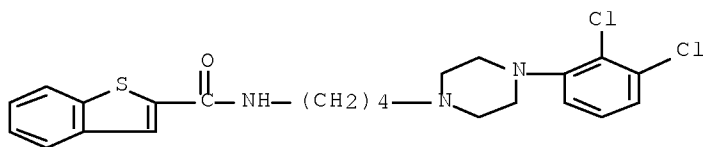
RN 474432-65-0 CAPLUS
 CN Benzo[b]thiophene-2-carboxamide, N-[4-[4-(2-methoxyphenyl)-1-

piperazinyl]butyl]- (CA INDEX NAME)



RN 474432-66-1 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 26 OF 31 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:541732 CAPLUS Full-text

DOCUMENT NUMBER: 129:230698

TITLE: Synthesis of new benzothienylpiperazine derivatives and their characterization at both 5HT1A and 5HT1B receptor sites

AUTHOR(S): Lamothe, M.; Pauwels, P. J.; Leborgne, M.; Halazy, S.
CORPORATE SOURCE: Medicinal Chemistry Division and Cellular, Centre de Recherche Pierre FABRE, CASTRES, 81106, Fr.

SOURCE: Medicinal Chemistry Research (1998), 8(3), 132-142
CODEN: MCREEB; ISSN: 1054-2523

PUBLISHER: Birkhaeuser Boston

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A new series of compds. containing a benzothienylpiperazine core and an arylpiperazine (or arylpiperidine) side chain has been prepared and evaluated as mixed 5HT1A and 5HT1B receptor antagonists. A SAR study allowed identification of one new compound as a new potent antagonist at both 5HT1A and 5HT1B receptor subtypes with Ki values in the nanomolar range.

IT 212901-61-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of benzothienylpiperazines as 5HT1A and 5HT1B receptor antagonist)

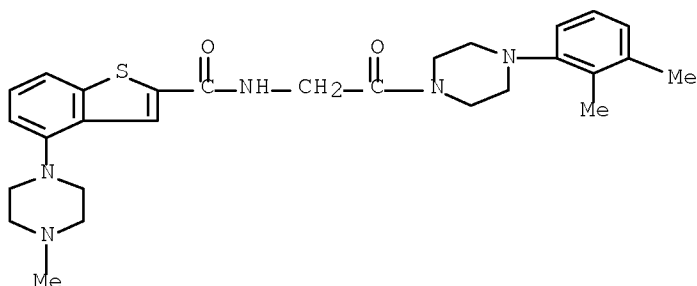
RN 212901-61-6 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, N-[2-[4-(2,3-dimethylphenyl)-1-piperazinyl]-2-oxoethyl]-4-(4-methyl-1-piperazinyl)-, (2E)-2-butenedioate (20:17) (CA INDEX NAME)

CM 1

CRN 186594-64-9

CMF C28 H35 N5 O2 S

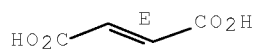


CM 2

CRN 110-17-8

CMF C4 H4 O4

Double bond geometry as shown.



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 27 OF 31 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1997:134916 CAPLUS Full-text
DOCUMENT NUMBER: 126:144292
TITLE: Novel heteroaromatic piperazines for use as drugs
INVENTOR(S): Halazy, Serge; Lamothe, Marie
PATENT ASSIGNEE(S): Pierre Fabre Medicament, Fr.; Halazy, Serge; Lamothe, Marie
SOURCE: PCT Int. Appl., 84 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 9641802	A1	19961227	WO 1996-FR853	19960606
W: AU, CA, JP, NZ, US				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
FR 2735127	A1	19961213	FR 1995-6825	19950609
FR 2735127	B1	19970822		
AU 9662296	A	19970109	AU 1996-62296	19960606

PRIORITY APPLN. INFO.:

FR 1995-6825

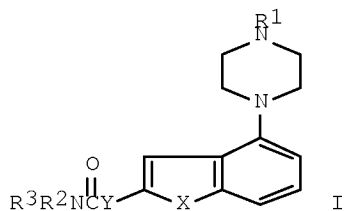
A 19950609

WO 1996-FR853

W 19960606

OTHER SOURCE(S):
GI

CASREACT 126:144292; MARPAT 126:144292



AB Title piperazines I [R^1 = H, C1-6 alkyl; X = O, S, NR^1 ; Y = various connecting groups; R^2 , R^3 = (same or different) H, alkyl, cycloalkyl, aryl, aralkyl], useful as inhibitors of cAMP, were prepared Thus, coupling 4-(2,3-dimethylphenyl)piperazine-HCl with [4-(4-methyl-1-piperazinyl)benzo[b]thiophen-2-yl]methanol in the presence of di-2-pyridyl carbonate and Et_3N in CH_2Cl_2 and then treating with fumaric acid gave I.fumarate [R^1 = Me; X = S; Y = OCH_2 ; NR^2R^3 = 4-(2,3-dimethylphenyl)-1-piperazinyl] which were tested for inhibitory activity in several human receptors.

IT 186594-65-0P 186595-59-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of piperazinyl-benzothiophenes, -benzofurans and -indoles as cAMP inhibitors)

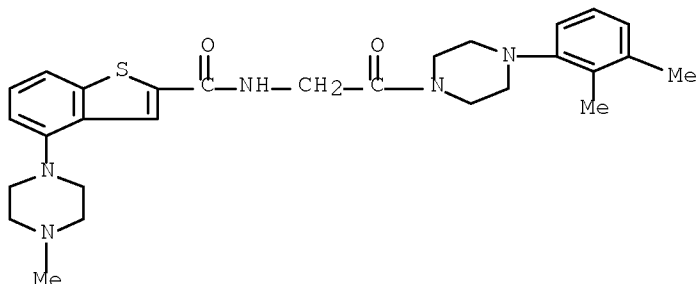
RN 186594-65-0 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, N-[2-[4-(2,3-dimethylphenyl)-1-piperazinyl]-2-oxoethyl]-4-(4-methyl-1-piperazinyl)-, (2E)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

CRN 186594-64-9

CMF C28 H35 N5 O2 S

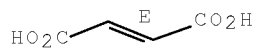


CM 2

CRN 110-17-8

CMF C4 H4 O4

Double bond geometry as shown.



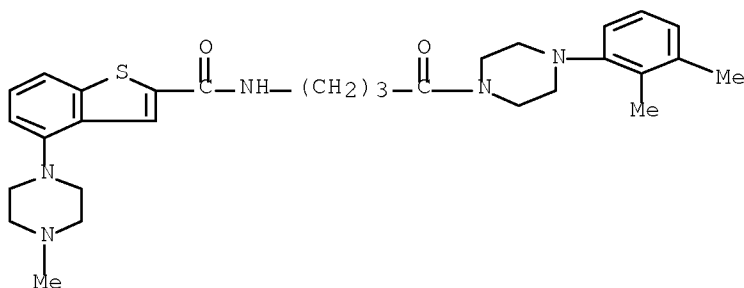
RN 186595-59-5 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, N-[4-[4-(2,3-dimethylphenyl)-1-piperazinyl]-4-oxobutyl]-4-(4-methyl-1-piperazinyl)-, (2E)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

CRN 186595-58-4

CMF C30 H39 N5 O2 S

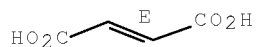


CM 2

CRN 110-17-8

CMF C4 H4 O4

Double bond geometry as shown.



L4 ANSWER 28 OF 31 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1992:504274 CAPLUS [Full-text](#)

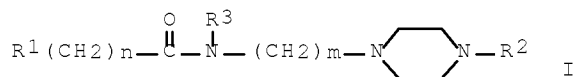
DOCUMENT NUMBER: 117:104274

TITLE: Use of aryl- and heteroaryl piperazinyl carboxamides in the treatment of anxiety, depression, and psychoses

INVENTOR(S): Abou-Gharbia, Magid A.; Yardley, John P.; Childers,

WAYNE E., JR.; MOYER, JOHN A.
 PATENT ASSIGNEE(S): American Home Products Corp., USA
 SOURCE: U.S., 12 pp. Cont.-in-part of U.S. 5,010,078.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5106849	A	19920421	US 1991-689409	19910422
ZA 8903836	A	19910130	ZA 1989-3836	19890522
US 5010078	A	19910423	US 1990-493179	19900314
US 5278160	A	19940111	US 1992-848782	19920310
US 5254552	A	19931019	US 1992-852119	19920316
US 5482940	A	19960109	US 1993-48088	19930415
US 5380725	A	19950110	US 1993-91495	19930714
PRIORITY APPLN. INFO.:			US 1988-197890	B2 19880524
			US 1989-297460	B2 19890113
			US 1990-493179	A2 19900314
			US 1989-335075	B2 19890407
			US 1990-533974	B1 19900606
			US 1991-689409	A3 19910422
			US 1992-848782	A3 19920310
			US 1992-852119	A3 19920316
OTHER SOURCE(S):			CASREACT 117:104274; MARPAT 117:104274	
			GI	



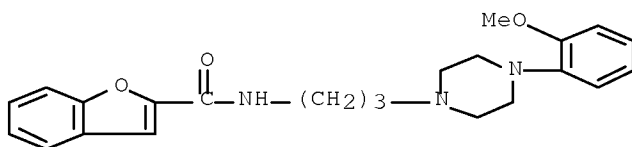
AB The title compds. I [R1 = 1-adamantyl, 3-methyl-1-adamantyl, 3-noradamantyl, etc.; R2 = (un)substituted Ph, benzyl, or pyrimidinyl; R3 = H, C1-3 alkyl; n = 0,1; m = 2-5] and their pharmaceutically acceptable salts are used in the treatment of anxiety, depression, and psychoses. Thus, N-[3-[4-(2-methoxyphenyl)-1-piperazinyl]propyl]- tricyclo[3.3.1.1.3,7]decane-1-carboxamide-HCl hemihydrate (preparation given) was evaluated for its binding of 5HT1A, 5HT2, and D2 receptors.

IT 127266-79-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, as central nervous system drug)

RN 127266-79-9 CAPLUS

CN 2-Benzofurancarboxamide, N-[3-[4-(2-methoxyphenyl)-1-piperazinyl]propyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

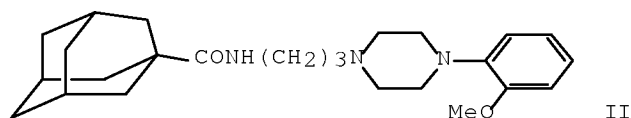
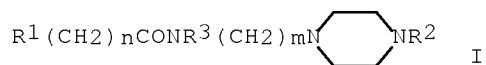
L4 ANSWER 29 OF 31 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1991:42811 CAPLUS Full-text
 DOCUMENT NUMBER: 114:42811
 TITLE: Preparation of N-[(4-aryl)piperazino]alkyl]adamantanecarboxamides and analogs as psychotropic agents
 INVENTOR(S): Abou, Gharbia Magid Abdel Megid; Yardley, John Patrick; Childers, Jr Wayne Everitt
 PATENT ASSIGNEE(S): American Home Products Corp., USA
 SOURCE: Brit. UK Pat. Appl., 39 pp.
 CODEN: BAXXDU
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 2218988	A	19891129	GB 1989-11912	19890524
GB 2218988	B	19911218		
IL 90279	A	19950330	IL 1989-90279	19890512
CA 1340113	C	19981103	CA 1989-599685	19890512
HU 53095	A2	19900928	HU 1989-2488	19890518
HU 205923	B	19920728		
FI 8902424	A	19891125	FI 1989-2424	19890519
FI 94130	B	19950413		
FI 94130	C	19950725		
AU 8935025	A	19891130	AU 1989-35025	19890522
AU 628341	B2	19920917		
ZA 8903836	A	19910130	ZA 1989-3836	19890522
DK 8902499	A	19891125	DK 1989-2499	19890523
DK 168665	B1	19940516		
JP 02015059	A	19900118	JP 1989-129975	19890523
KR 128345	B1	19980403	KR 1989-6857	19890523
EP 343961	A2	19891129	EP 1989-305255	19890524
EP 343961	A3	19910116		
EP 343961	B1	19960110		
R: AT, BE, CH, DE, ES, FR, GR, IT, LI, LU, NL, SE				
AT 132862	T	19960115	AT 1989-305255	19890524
ES 2081302	T3	19960301	ES 1989-305255	19890524
US 5254552	A	19931019	US 1992-852119	19920316
US 5380725	A	19950110	US 1993-91495	19930714
PRIORITY APPLN. INFO.:			US 1988-197890	A 19880524
			US 1989-297460	A 19890113
			US 1989-335075	B2 19890407
			US 1990-493179	A3 19900314
			US 1990-533974	B1 19900606

OTHER SOURCE(S):

CASREACT 114:42811; MARPAT 114:42811

GI



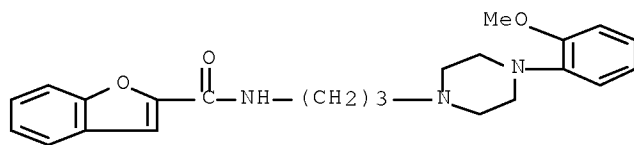
AB The title compds. [I; R¹ = 1-adamantyl, 3-methyl-1-adamantyl, 3-noradamantyl, (un)substituted 2- or 3-indolyl, 2- or 3-benzofuranyl; R² = (un)substituted Ph, PhCH₂, pyridyl, pyrimidinyl, pyrazinyl; R³ = H, alkyl; n = 0, 1; m = 2-5] were prepared. Thus, 3-[4-(2-methoxyphenyl)piperazino]propylamine was stirred overnight with adamantane-1-carboxylic acid chloride to give title compound II as the hydrochloride which had K_i of 1 nM for 5-HT_{1A} receptor affinity.

IT 127266-60-8P 127266-79-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as psychotropic agent)

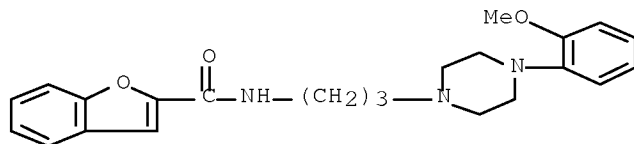
RN 127266-80-8 CAPLUS

CN 2-Benzofurancarboxamide, N-[3-[4-(2-methoxyphenyl)-1-piperazinyl]propyl]-
(CA INDEX NAME)



RN 127266-79-9 CAPLUS

CN 2-Benzofurancarboxamide, N-[3-[4-(2-methoxyphenyl)-1-piperazinyl]propyl]-, dihydrochloride (9CI) (CA INDEX NAME)



L4 ANSWER 30 OF 31 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1973:442558 CAPLUS Full-text

DOCUMENT NUMBER: 79:42558

ORIGINAL REFERENCE NO.: 79:6925a,6928a

TITLE: N-[-(4-phenyl-1-piperazinyl)alkyl]benzo[b]thiophene or benzofuran-2-carboxamides

INVENTOR(S): Wright, William Blythe, Jr.; Brabander, Herbert Joseph

PATENT ASSIGNEE(S): American Cyanamid Co.

SOURCE: U.S., 4 pp. Continuation-in-part of U.S. 3,646,047 (CA 76;140541w).

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3734915	A	19730522	US 1971-189727	19711015
US 3646047	A	19720229	US 1970-8090	19700202
PRIORITY APPLN. INFO.:			US 1970-8090	A2 19700202

GI For diagram(s), see printed CA Issue.

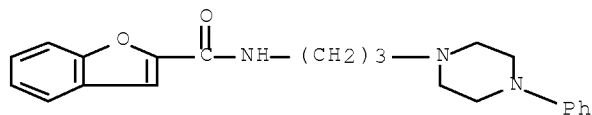
AB Piperazinylbenzothiophene- or -benzofurancarboxamides (I, R = R1 = H, Cl, R = Cl, R1 = H; X = O, S; n = 2, 3) were prepared Thus, benzo[b]thiophene-2-carbonyl chloride was treated with Br(CH2)3NH2 to give N-(3-bromopropyl)benzo[b]thiophene-2-carboxamide which was treated with 1-phenylpiperazine to give I (R = R1 = H, X = S, n = 3). I are central nervous depressants and analgesics.

IT ~~36158-03-9P 36158-04-0P 36175-20-9P~~
~~36175-21-0P 36175-23-2P 36175-24-3P~~
~~36175-26-5P 36175-27-6P 36175-28-7P~~
~~36410-63-6P~~

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

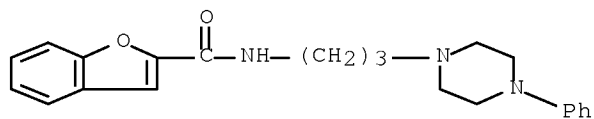
RN 36158-03-9 CAPLUS

CN 2-Benzofurancarboxamide, N-[3-(4-phenyl-1-piperazinyl)propyl]- (CA INDEX NAME)



RN 36158-04-0 CAPLUS

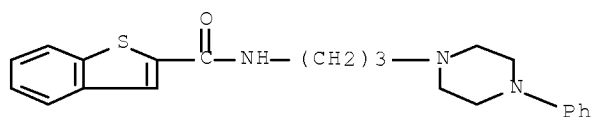
CN 2-Benzofurancarboxamide, N-[3-(4-phenyl-1-piperazinyl)propyl]-, hydrochloride (9CI) (CA INDEX NAME)



●x HCl

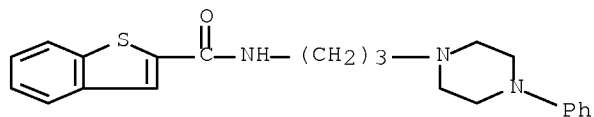
RN 36175-20-9 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, N-[3-(4-phenyl-1-piperazinyl)propyl]-
(CA INDEX NAME)



RN 36175-21-0 CAPLUS

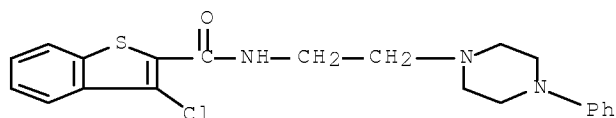
CN Benzo[b]thiophene-2-carboxamide, N-[3-(4-phenyl-1-piperazinyl)propyl]-,
hydrochloride (9CI) (CA INDEX NAME)



●x HCl

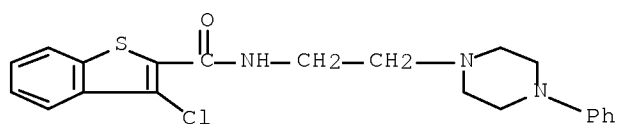
RN 36175-23-2 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, 3-chloro-N-[2-(4-phenyl-1-piperazinyl)ethyl]-
(CA INDEX NAME)



RN 36175-24-3 CAPLUS

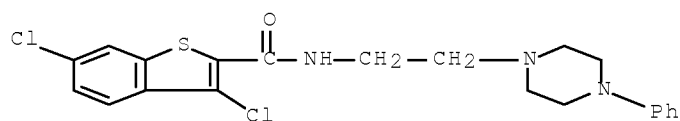
CN Benzo[b]thiophene-2-carboxamide, 3-chloro-N-[2-(4-phenyl-1-piperazinyl)ethyl]-,
hydrochloride (9CI) (CA INDEX NAME)



●x HCl

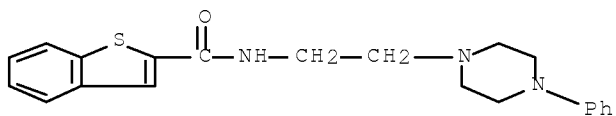
RN 36175-26-5 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, 3,6-dichloro-N-[2-(4-phenyl-1-piperazinyl)ethyl]- (CA INDEX NAME)



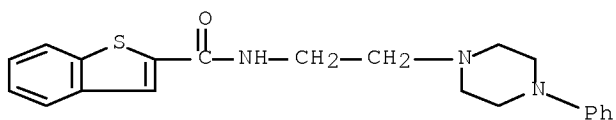
RN 36175-27-6 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, N-[2-(4-phenyl-1-piperazinyl)ethyl]- (CA INDEX NAME)



RN 36175-28-7 CAPLUS

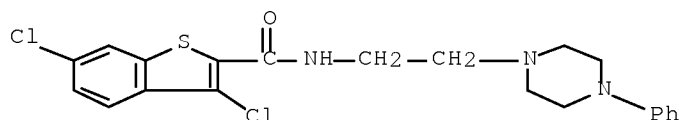
CN Benzo[b]thiophene-2-carboxamide, N-[2-(4-phenyl-1-piperazinyl)ethyl]-, hydrochloride (9CI) (CA INDEX NAME)



●x HCl

RN 36410-63-6 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, 3,6-dichloro-N-[2-(4-phenyl-1-piperazinyl)ethyl]-, hydrochloride (9CI) (CA INDEX NAME)

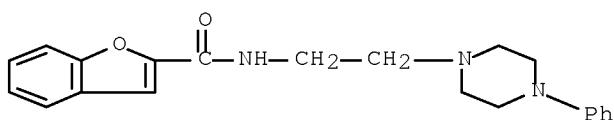


●x HCl

L4 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1972:140541 CAPLUS Full-text
 DOCUMENT NUMBER: 76:140541
 ORIGINAL REFERENCE NO.: 76:22807a,22810a
 TITLE: Pharmacologically active benzo[b]thiophene-2-carboxamide derivatives
 INVENTOR(S): Wright, William Blythe, Jr.; Brabander, Herbert J.
 PATENT ASSIGNEE(S): American Cyanamid Co.
 SOURCE: U.S., 5 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3646047	A	19720229	US 1970-8090	19700202
US 3734915	A	19730522	US 1971-189727	19711015
PRIORITY APPLN. INFO.:			US 1970-8090	A2 19700202

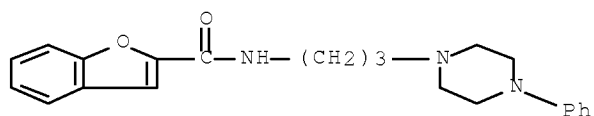
GI For diagram(s), see printed CA Issue.
 AB Carboxamides (I, X = S, O, n = 2, 3, R1, R2 = H, Cl, R3 = 4-phenylpiperidino, 4-phenyl-1-piperazinyl, 5,6-dihydro-4-phenyl-1(2H)-pyridyl) were prepared E.g., treatment of 2-benzo-furancarboxylic acid and N,N'-carbonyl-1-diimidazole with 2-(4-phenyl-1-piperazinyl)ethylamine gave N-[2-(4-phenyl-1-piperazinyl)ethyl]-2-benzofurancarboxamide (I, X = O, n = 2, R1 = R2 = H, R3 = 4-phenyl-1-piperazinyl) (II). Similarly prepared were 16 addnl. I. In mice, II was an analgesic at 200 mg/kg and a tranquilizer at 9 mg/kg.
 IT 36158-02-8P 36158-03-9P 36158-04-0P
 36175-20-9P 36175-21-0P 36175-23-2P
 36175-24-3P 36175-26-5P 36175-27-6P
 36175-28-7P 36175-34-5P 36410-63-6P
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)
 RN 36158-02-8 CAPLUS
 CN 2-Benzofurancarboxamide, N-[2-(4-phenyl-1-piperazinyl)ethyl]-, hydrochloride (9CI) (CA INDEX NAME)



●x HCl

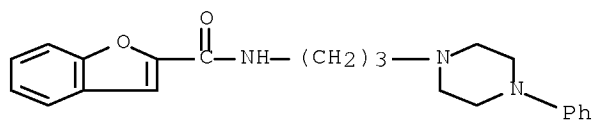
RN 36158-03-9 CAPLUS

CN 2-Benzofurancarboxamide, N-[3-(4-phenyl-1-piperazinyl)propyl]- (CA INDEX NAME)



RN 36158-04-0 CAPLUS

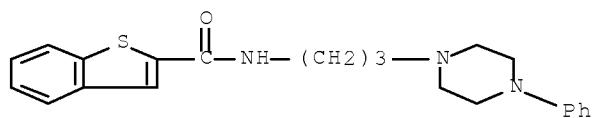
CN 2-Benzofurancarboxamide, N-[3-(4-phenyl-1-piperazinyl)propyl]-, hydrochloride (9CI) (CA INDEX NAME)



●x HCl

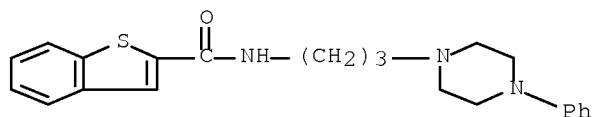
RN 36175-20-9 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, N-[3-(4-phenyl-1-piperazinyl)propyl]- (CA INDEX NAME)



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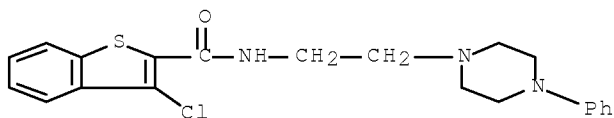
CN Benzo[b]thiophene-2-carboxamide, N-[3-(4-phenyl-1-piperazinyl)propyl]-, hydrochloride (9CI) (CA INDEX NAME)



●x HCl

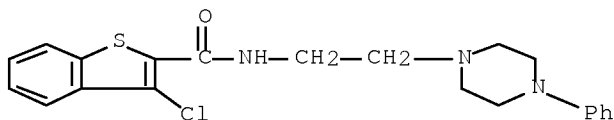
RN 36175-23-2 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, 3-chloro-N-[2-(4-phenyl-1-piperazinyl)ethyl]- (CA INDEX NAME)



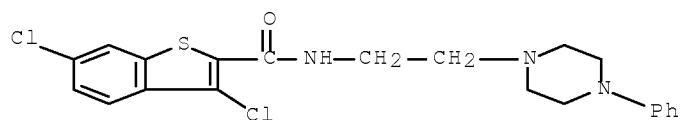
RN 36175-24-3 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, 3-chloro-N-[2-(4-phenyl-1-piperazinyl)ethyl]-, hydrochloride (9CI) (CA INDEX NAME)



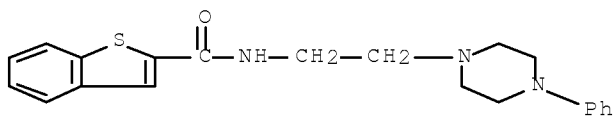
RN 36175-26-5 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, 3,6-dichloro-N-[2-(4-phenyl-1-piperazinyl)ethyl]- (CA INDEX NAME)



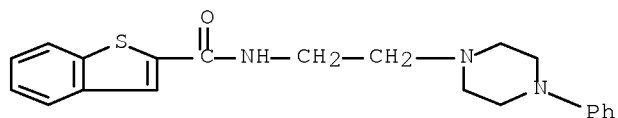
RN 36175-27-6 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, N-[2-(4-phenyl-1-piperazinyl)ethyl]- (CA INDEX NAME)



RN 36175-28-7 CAPLUS

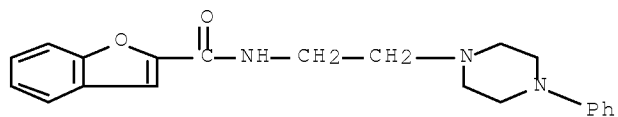
CN Benzo[b]thiophene-2-carboxamide, N-[2-(4-phenyl-1-piperazinyl)ethyl]-,
hydrochloride (9CI) (CA INDEX NAME)



●x HCl

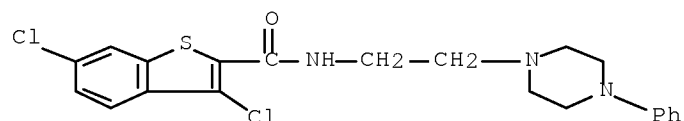
RN 36175-34-5 CAPLUS

CN 2-Benzofurancarboxamide, N-[2-(4-phenyl-1-piperazinyl)ethyl]- (CA INDEX
NAME)



RN 36410-63-6 CAPLUS

CN Benzo[b]thiophene-2-carboxamide, 3,6-dichloro-N-[2-(4-phenyl-1-
piperazinyl)ethyl]-, hydrochloride (9CI) (CA INDEX NAME)



●x HCl

=> d his

(FILE 'HOME' ENTERED AT 09:38:21 ON 07 FEB 2008)

FILE 'REGISTRY' ENTERED AT 09:38:26 ON 07 FEB 2008

L1 STRUCTURE UPLOADED

L2 4 S L1

L3 91 S L1 FULL

FILE 'CAPLUS' ENTERED AT 09:40:06 ON 07 FEB 2008

L4 31 S L3 FULL

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COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	172.31	351.80
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-24.80	-24.80

STN INTERNATIONAL LOGOFF AT 09:44:22 ON 07 FEB 2008